

**Φ ULVAC-PHI, INC.**

**OPERATOR'S  
PHI MultiPak™  
Software Manual  
VERSION 9**

Part No. 706704 Rev. K

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# ULVAC-PHI Safety Notices

ULVAC-PHI's products are designed and manufactured in compliance with accepted worldwide practices and standards to provide protection against electrical and mechanical hazards for the operator and the area surrounding the product. All ULVAC-PHI's products are designed and intended for professional use only, by skilled "operators" for their intended purpose and according to all of the instructions, safety notices, and warnings provided by ULVAC-PHI.

Those instructions, notices, and warnings assume that an "operator" will not employ any tool when using ULVAC-PHI products. They further assume that all operators clearly understand that use of ULVAC-PHI products in any manner not specified by ULVAC-PHI may impair the protection provided by the products and expose them to hazards.

A "technician" is a qualified servicing individual who:

- Has received training to work with voltages above 50 V,
- Has read and understood the ULVAC-PHI technician's manual for the equipment,
- Observes and understands all safety notices on ULVAC-PHI equipment.

The safety symbols that ULVAC-PHI uses are defined on the following page.\* To reduce or eliminate hazards, technicians and operators of this equipment must fully understand these symbols.

ULVAC-PHI's products are installed with international-style or ANSI†-style safety notices, according to site requirements. International notices are symbols within triangles (alerts) or circles (mandatory actions). ULVAC-PHI's ANSI-style safety notices contain:

- One of three signal words (in all capitals) preceded by the general caution symbol ();
  - One of ULVAC-PHI's safety symbols along with a brief description of the hazard and the risk or injury that could occur;
  - Short message that observes ANSI's Hazard Alert Trilogy Rule by identifying the hazard, the possible result of ignoring the notice, and how to avoid the hazard.
- The three signal words are defined as follows:
- **DANGER**—imminently hazardous situation that, if not avoided, will result in death or serious injury;
  - **WARNING**—potentially hazardous situation that, if not

avoided, could result in death or serious injury;

- **CAUTION**—potentially hazardous situation or unsafe practice that, if not avoided, may result in minor or moderate injury or damage to equipment.

SEMI‡ standards require identification of type 3, 4, and 5 electrical maintenance tasks in equipment manuals:

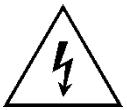
- **Type 3** electrical maintenance tasks involve energized equipment, exposed live circuits, and possible accidental contact; potential exposures are less than 30 V RMS, 42.2 V peak, 240 V-A, and 20 J.
- **Type 4** is the same but potential exposures are greater than 30 V RMS, 42.2 V peak, 240 V-A, and 20 J or radio frequency is present.
- **Type 5** tasks involve energized equipment and measurements and adjustment require physical entry into the equipment, or equipment configuration will not allow the use of clamp-on probes.

Only experienced, trained technicians should attempt to perform type 3, 4, or 5 electrical maintenance tasks.

\* Many of ULVAC-PHI's safety symbols are provided and copyrighted by Clarion Safety Systems LLC, Milford, PA.

† American National Standards Institute, 1430 Broadway, New York, NY 10018.

‡ Semiconductor Equipment and Materials International, 805 E. Middlefield Rd., Mountain View, CA 94043-4080.



Voltages may be present that could cause death or personal injury.



Caution (General risk). Refer to the manual(s) before proceeding.



Pulling the plug from its power source before servicing is mandatory.



A pinching point is present that could cause personal injury.



A risk of explosion or implosion may be present that could cause personal injury.



Lifting with assistance or equipment could cause personal injury.



An overhead door is present that could cause personal injury. Do not work under door without auxiliary door supports installed.



Visible or invisible radiation may be present that could cause personal injury.



Hot surfaces may be present that could cause personal injury.



Turning off the power switch before servicing is mandatory.



Refer to the manual(s) before proceeding.



Contents are under pressure.



A harmful or irritant material may be present that could cause personal injury.



Extremely low temperatures may be present that could cause personal injury.



A risk of fire may be present that could cause personal injury.



A potentially dangerous magnetic field may be present.



An environment with depleted oxygen may be present that could cause death or personal injury. Open at least 2 doors and wait 2 minutes before entering the enclosure.



Wearing protective gloves is mandatory.



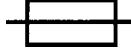
Wearing eye protection is mandatory.



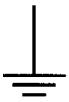
Wearing foot protection is mandatory.



This is the location of the protective grounding conductor terminal.



This is the location of the fuse.



This is the location of an earth (ground) terminal.

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# Limited Warranty

---

Except as otherwise provided herein, the Seller warrants to Buyer that the equipment sold hereunder, whether it is new equipment or remanufactured (reconditioned) equipment, is, at the time of shipment to Buyer from Seller, free from defects in material and workmanship. As Buyer's sole exclusive remedy under this warranty Seller agrees either to repair or replace, at Seller's sole option and free of part charge to Buyer, any part or parts of such equipment which, under proper and normal conditions of use prove to be defective within 12 months from the date of receipt by the Buyer. Warranty period for equipment requiring installation by Seller will commence on completion of standard installation services. If customer delays installation beyond 45 days after delivery, the warranty period will commence to run 45 days after delivery. After installation, any realignment, readjustment, recleaning or recalibration, provided it does not relate to a proven defect in material or workmanship, shall be performed only at Seller's then current rates for service.

## ***Exclusions and Limitations***

It is recognized that some parts by their nature (expendable items) may not function for one full year; therefore, excluded from the foregoing warranty are filaments, anodes, cathodes, multipliers, retard grids, special ceramics, ionizers, along with other such parts mentioned in the applicable operating manual.

The foregoing warranty excludes certain major items or accessories specifically indicated on applicable price lists or quotations, as to which Seller passes to Buyer whatever warranty is provided to Seller by the manufacturer or the

specific warranty indicated by the price list or quotation.

This warranty does not cover loss, damage, or defects resulting from transportation to the Buyer's facility, improper or inadequate maintenance by Buyer, buyer-supplied software or interfacing, unauthorized modification or misuse, operation outside of the environmental specifications for the equipment or improper site preparation and maintenance.

## ***Product Service***

All claims must be brought to the attention of Seller within 30 days of the failure to perform.

Seller at his option may require the product to be returned to the factory, transportation prepaid, for repair.

## ***Refund of Purchase Price***

In lieu of the foregoing, Seller may at any time elect, in its sole discretion, to discharge its warranty by accepting the return of such equipment and refunding any portion of the purchase price paid by Buyer.

## ***Software and Firmware Products***

The sole exclusive warranty applicable to software and firmware products provided by Seller for use with a processor will be as follows: Seller warrants that such software and firmware will conform to Seller's program manuals current at the time of shipment to Buyer when properly installed on that processor. Seller does not warrant that the operation of the processor software or firmware will be uninterrupted or error free.

No other warranty is expressed or implied. Seller expressly disclaims the implied warranties of merchantability and fitness for a particular purpose.

# **Section 1:**

## **Introduction and Overview**

---

MultiPak™ is ULVAC-PHI' (PHI's) software for extensive data interpretation and complex image processing of Auger and ESCA / XPS data acquired with PHI systems or software. MultiPak operates on IBM-compatible PCs on PHI systems, and on IBM-compatible PCs as a standalone package for off-line analysis of data acquired with PHI systems or software.

MultiPak works with data files created in PHI *SmartSoft™*, PHI *COMPASS™*; and MultiPak clone files created in PHI *ACCESS™*, PHI *PC-ACCESS™*, PHI *PC-EXPLORER™*, and PHI *SUMMITT™* data acquisition software.

## **Computer Requirements**

Computer requirements for MultiPak in a PC environment are the following:

Operating system: Windows® XP SP3/Windows 7™ (32bit);

- CPU: IBM PC® compatible Pentium® 4 3.8 G MHz or Core™2 Duo 2.66GHz or Higher recommended;
- RAM (Random Access Memory): 1 GB minimum, 2 GB recommended;
- Monitor: graphics accelerator recommended; 1280×1024 Full-Color;
- Hard-disk free space:
  - 1 GB for MultiPak;
  - 3.0 MB for AES handbook data;
  - 3.1 MB for XPS handbook data;
  - Space for data files, which can vary in size from 2 KB for a single survey spectrum to many tens of megabytes for multiple-element, high-pixel-density images;
- CD-ROM Drive

PHI-supplied PCs are typically equipped with a minimum hard drive capacity of 20 GB.

## How To Use This Manual

This manual is presented in three sections:

- Section 1 describes MultiPak's relationship to other ULVAC-PHI products and its computer requirements and describes the primary characteristics of MultiPak's user interface: windows, functions, and mouse operations.
- Section 2 describes installing and starting MultiPak, describes Windows features like menus, buttons and check boxes, and walks through typical AES and XPS data reduction sequences.
- Section 3 contains detailed reference information about MultiPak functions.

*NOTE: Topics specific to the operating system (Windows) of the computer on which MultiPak is running are not covered in this manual, but may be explained in the documentation for your operating system.*

The manual also has four appendices:

- Appendix A briefly describes certain mathematical algorithms for data reduction used in MultiPak.
- Appendix B and C list the XPS Sensitivity Factors and AES Sensitivity Factors, respectively, used in MultiPak's elements database.
- Appendix D describes how to translate and transfer data files from an Apollo computer to a PC for use in MultiPak.

## MultiPak Windows

MultiPak has four main windows: the Spectrum, Profile, and Map windows, which are very similar in appearance and layout, and the Periodic Table window.

At startup, the Spectrum window is displayed on the left side of the desktop and the Periodic Table window is displayed on the right. When opened, the Profile and Map windows are displayed on the right side of the desktop screen. The Profile and Map windows will be displayed on top of the Periodic Table window. (Another MultiPak window can be moved to the foreground by selecting its name from the Window menu of any MultiPak window.)

The extension of the file name determines which window a data file will open in, as follows:

- **Spectrum Window**—files having the SPE (spectral data) extension. SPE files contain survey and multiplex acquisitions. Surveys are scans performed over certain energy ranges to identify the primary elements present in a sample. Multiplexes are scans that contain multiple regions.

- **Profile Window**—files having the PRO (depth profiles), ANG (angular profiles), or LIN (line scans) extensions (plus associated spectra in the Spectrum window). Depth profiles are performed to obtain compositional data as a function of sample depth. Angle profiles are ESCA acquisitions that provide a nondestructive depth profile of the near-surface region. Line profiles provide the surface distribution of an element along a straight line. A line profile is collected point by point over the defined line.
- **Map Window**—files having the MAP (map images), SEM (scanning electron micrographs), BSE (backscattered electron image), ABS (absorbed current image), SXI (secondary-electron x-ray induced image), and PHO (digital photographic images) extensions, plus associated displays in the Spectrum window). MAP files provide information on the two-dimensional surface distribution of an element. Map data is collected point by point in a grid fashion over a selected area of the sample. SEM, BSE, and ABS files are AES image acquisitions. SXI and PHO files are ESCA image acquisitions.

Each window has a menu bar, upper and lower toolbar, region bar, a header area, and a status bar (Figure 1-1), as described in the following subsections.

*NOTE: Use the tutorials in Section 2 to learn more about any terms used below that are unfamiliar.*

### **Menus, Selecting Functions, and Other Windows Terminology**

MultiPak's three main windows (Spectrum, Profile, and Map) use the same seven “main menus” on their menu bars: File, Edit, View, Tools, Data, Window, and Help. A MultiPak function is started (“selected”) by finding it on a menu or an associated cascading “submenu,” then highlighting it and releasing the mouse button, as illustrated in Figure 1-2. Many functions can also be started using short-cut keys (shown on the menus) or clicking on (“pressing”) a pushbutton in the upper toolbar.

Parameters for a function are set by the operator using a dialog box or the lower toolbar. Common features of these—“option menus,” buttons, and boxes—are illustrated in Figure 1-3. Other menu items are followed by an ellipse (...), such as Print (“Print...”) on the File menu, meaning that a dialog box will open when the menu item is selected.

### **Toolbars and Region Bar**

As shown in Figure 1-1, MultiPak has three toolbars: the upper toolbar, the lower toolbar, and the region bar. A toolbar is a portion of a window that contains “buttons” that can be used to perform many functions in MultiPak.

The upper toolbar is located below the window's menu bar and above the data display area of the window. The lower toolbar is located below the data display area and above the region bar. The region bar is located below the lower toolbar and above the status bar.

## 1: Introduction and Overview

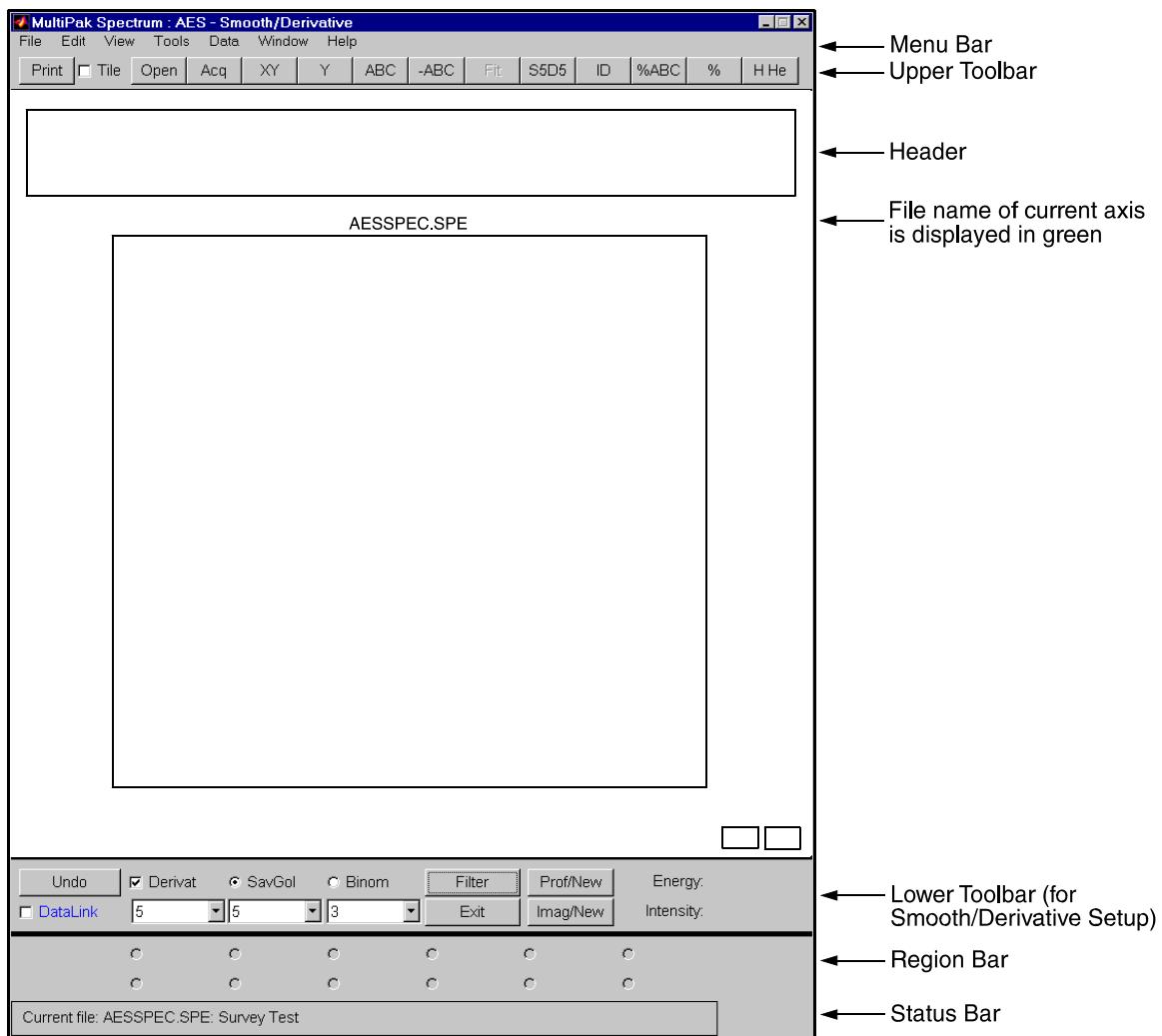


Figure 1-1. Parts of the MultiPak Window.

### Header

The header, displayed above the data's axes, is the listing of parameters from the currently selected data file.

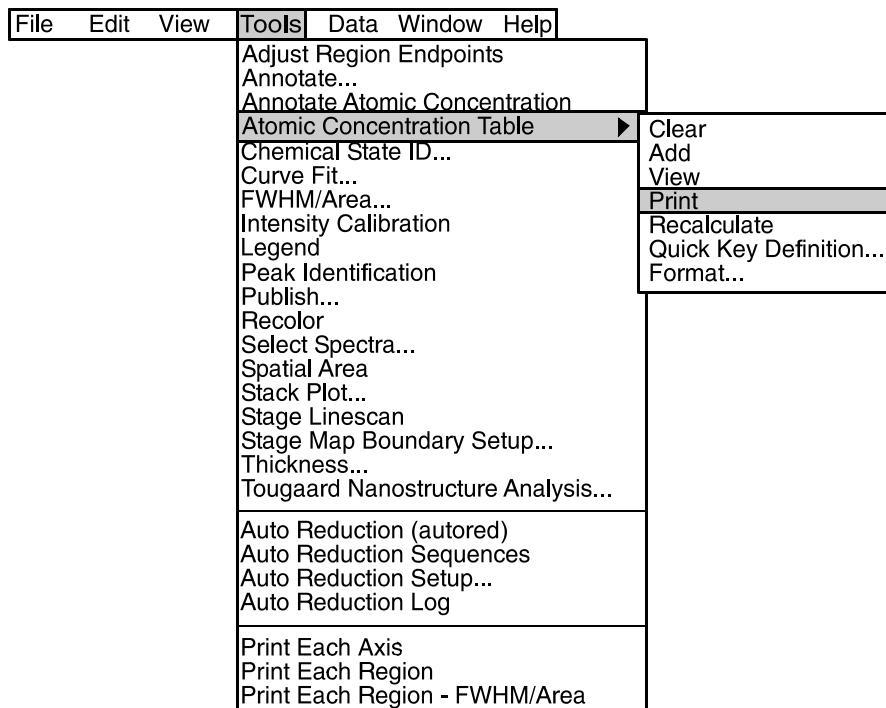
### Status Bar

The status bar, located at the bottom of the window, is used to display operator messages, system notices, and the name of the currently selected file.

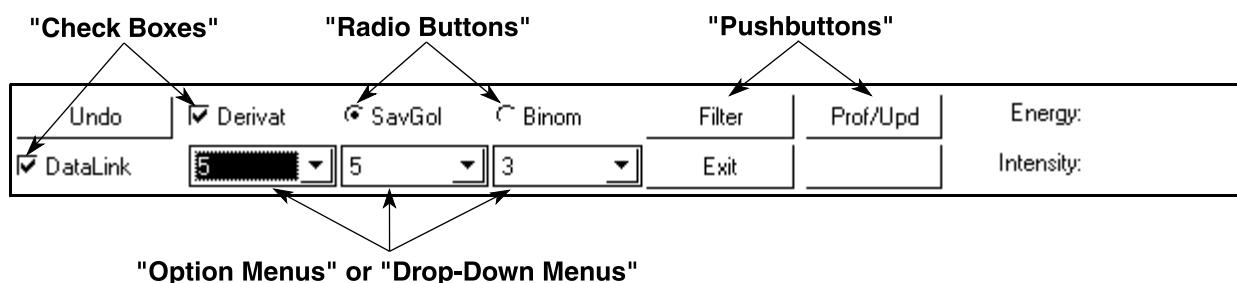
### Current or Selected Data

When multiple sets of data are displayed in a window, a green title above a set of data indicates that it is the currently selected data. The file name of the selected data set is also displayed in the status bar at the bottom of the window. Data are selected using the left mouse button.

## 1: Introduction and Overview



*Figure 1-2.* Selecting a Function from a Cascading Menu:  
"Select Tools—Atomic Concentration Table—Print."



**Check boxes** are toggle switches that are on when filled and off when not filled.

A **radio button** is one button in a set of buttons, only one of which can be on at a time. A button is on when filled and off when not filled.

A **pushbutton** activates a function. To "press" a button, click on it once with the left mouse button.

**Option menus** are **drop-down menus** that are displayed by clicking the arrow. An item is selected from the menu by clicking on it when the drop-down menu is displayed.

*Figure 1-3.* Buttons, Check Boxes, and Option/Drop-Down Menus.

## **1: Introduction and Overview**

Most functions, when activated, are applied to the current spectrum or image only. Further, many functions will retain their last setting indefinitely, so that displays of newly opened spectra or images will be based on that setting.

In this manual, the terms “current,” “selected,” and “currently selected” are all used.

### ***Formats for Viewing Multiple Axes***

Four formats are available for viewing multiple axes in a single window at the same time. Up to 36 axes (six rows and six columns) can be displayed concurrently in three of the views: *Landscape* (oriented in rows first, then columns); *Portrait* (oriented in columns first, then rows); and *Square* (landscape arrangement but all axes are equal in size). Up to 6 axes can be displayed concurrently in the *Stack* view (stacked in six rows in one column).

## **MultiPak’s Menus and Mouse Functions at a Glance**

The PC versions of MultiPak’s menus are shown in Figures 1-4 through 1-7. The ESCA menus are shown. The AES menus are virtually identical. (Differences are listed in the figure captions.) Tables 1-1 through 1-5 give a quick glance at mouse operations in the windows. (Mouse operations can also be listed by selecting Mouse from the Help menu.)

## 1: Introduction and Overview

Table 1-1. Mouse Functions Common to the **Spectrum, Profile, and Map** Windows.

To:	Point At:	Press:
Display and/or select menu items	menu item	Left or Left & drag
Display and/or select data	data or x or y axis	Left
Turn button on and off ("toggle")	button	Left
See all open files or only the selected one	Tile check box on the upper toolbar	Left
Write the display inside the window to a word processing file	Edit–Copy To Clipboard	Left
Print the display inside the window to a black and white or color printer or to a file	Print on the upper toolbar, or File–Print in B+W, File–Print in Color, or File–Print...	Left
View or change the data parameters listed in the header	File–Data Parameters–View	Left
Change the identification listed in the header	File–Options–System Settings...	Left *
Add annotation	1. Tools–Annotate or ABC pushbutton on the upper toolbar 2. Inside data area where the text is to be placed	1. Left * 2. Left
Move annotation	annotation within the x and y axes	Left & drag
Remove individual annotation	annotation within the x and y axes	Left & drag outside the data area
Duplicate last typed or highlighted annotation	Text to be duplicated	Right & drag
Export selected data as a graphics file	File–Export To–<file format>	Left *
View and/or change data, region, axis, or transition properties	data, region cursor, x or y axis, or periodic table element, respectively	[Shift]-Left *
View and/or change font, size, color, and/or orientation of annotation	annotation within the x and y axes	[Shift]-Left
View or change transmission function correction coefficient	Tools–Intensity Calibration–Update File... (ESCA files only)	Left *
Save the data inside the window in ASCII format	File–Export To–ASCII	Left

\* Pressing this mouse button displays additional options. See the function in Section 3 for details.

## 1: Introduction and Overview

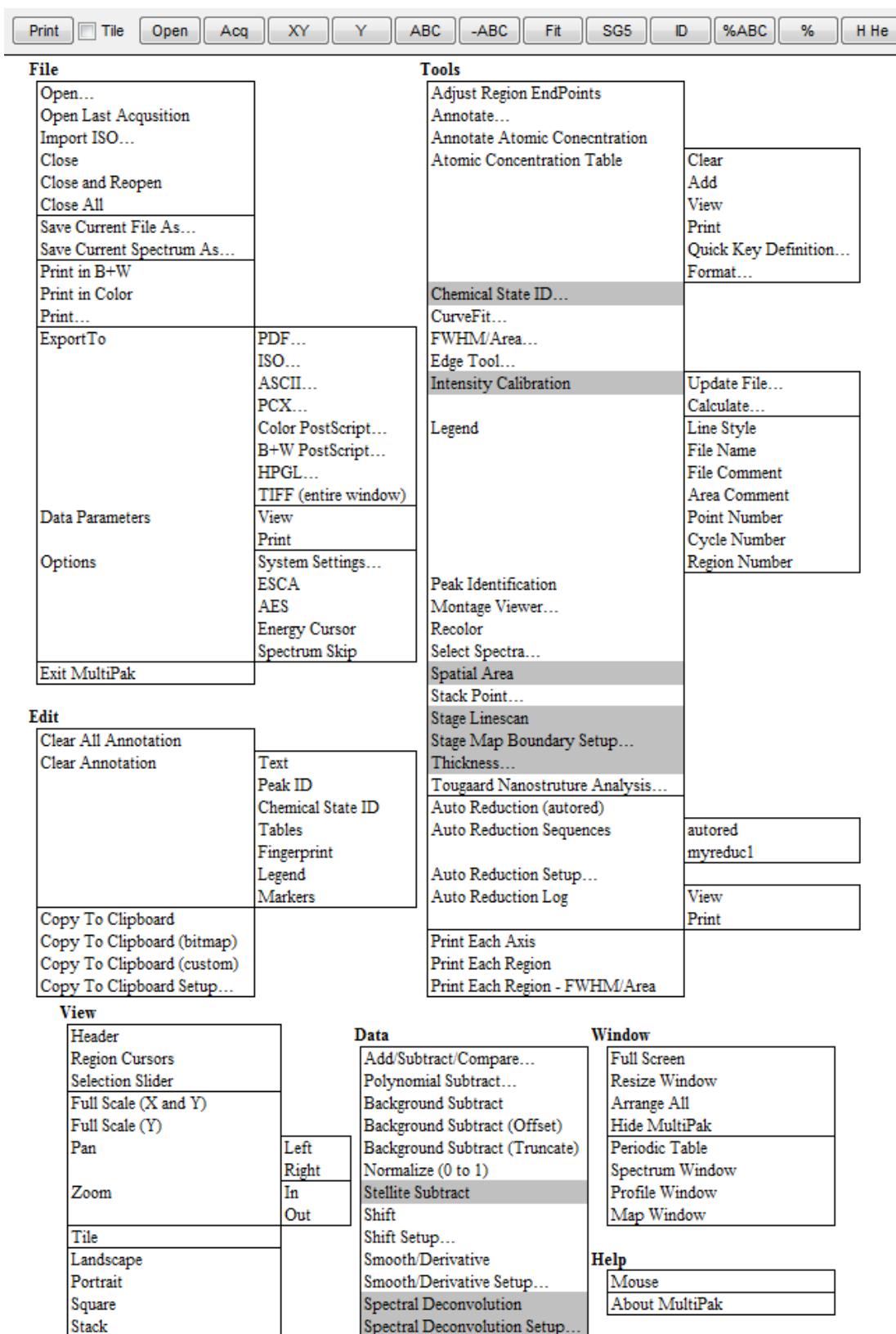


Figure 1-4. Menus and Upper Toolbar in the ESCA Spectrum Window.  
(The shaded functions are not available in the AES Spectrum window.)

## 1: Introduction and Overview

Table 1-2. Mouse Functions in the **Spectrum** Window.

To:	Point At:	Press:
Expand (zoom in to) region	region button in region bar	Left
Expand (zoom in to) horizontal, vertical, or diagonal subregion	anywhere within current x and y axes	Left & drag
Show whole spectrum	active region button in region bar or XY pushbutton in upper toolbar	Left
Show full spectrum intensity	Y pushbutton in upper toolbar	Left
Display transition peak labels (using "energy cursor") and annotate spectrum with labels	anywhere within current x and y axes	Right & drag
Display transition peak labels (using "energy cursor") but do not annotate with labels	anywhere within current x and y axes	[Shift]-Left & drag
Move a region boundary	region boundary	Left & drag
Move region boundaries without changing the width of the region	region boundary	Right & drag
View and/or change intensity calculation method or background calculation method	region boundary	[Shift]-Left *
View lower and upper x coordinates of the region	region or subregion boundary	[Shift]-Left *
View and/or change axis titles and/or axis start and end points	x or y axis	[Shift]-Left *
Change the arrangement of multiple displays	View–Landscape, –Portrait, –Square, or –Stack	Left
Scroll left and right along the spectrum	View–Pan or drag energy cursor or region cursor outside left or right axis	Left
Automatically generate atomic concentration table	% on the upper toolbar (Atomic Concentration Table 'Quick Key')	Left
Automatically add AC table data to the spectrum	%ABC pushbutton on the upper toolbar	Left
Normalize all spectra for data comparison	Data–Normalize	Left
Select smoothing and/or differentiation algorithms	Data–Smooth/Derivative Setup...	Left *
Perform preselected smooth/differentiation algorithms	SGn, SnDn, or Binom pushbutton on upper toolbar	Left
Shift data to align a specific peak	Data–Shift Setup...	Left *
Label known transition peaks on the spectrum	ID pushbutton on the upper toolbar	Left
Compute height, energy, area, FWHM, and background noise of region	Tools–FWHM/Area...	Left *
Create profiles from a series of spectra	Prof/New or Prof/Upd pushbutton on the lower toolbar	Left
Perform nonlinear curve fit on data (ESCA only)	Tools–Curve Fit, or Fit pushbutton on the upper toolbar	Left *

\* Pressing this mouse button displays additional options. See the function in Section 3 for details.

## 1: Introduction and Overview

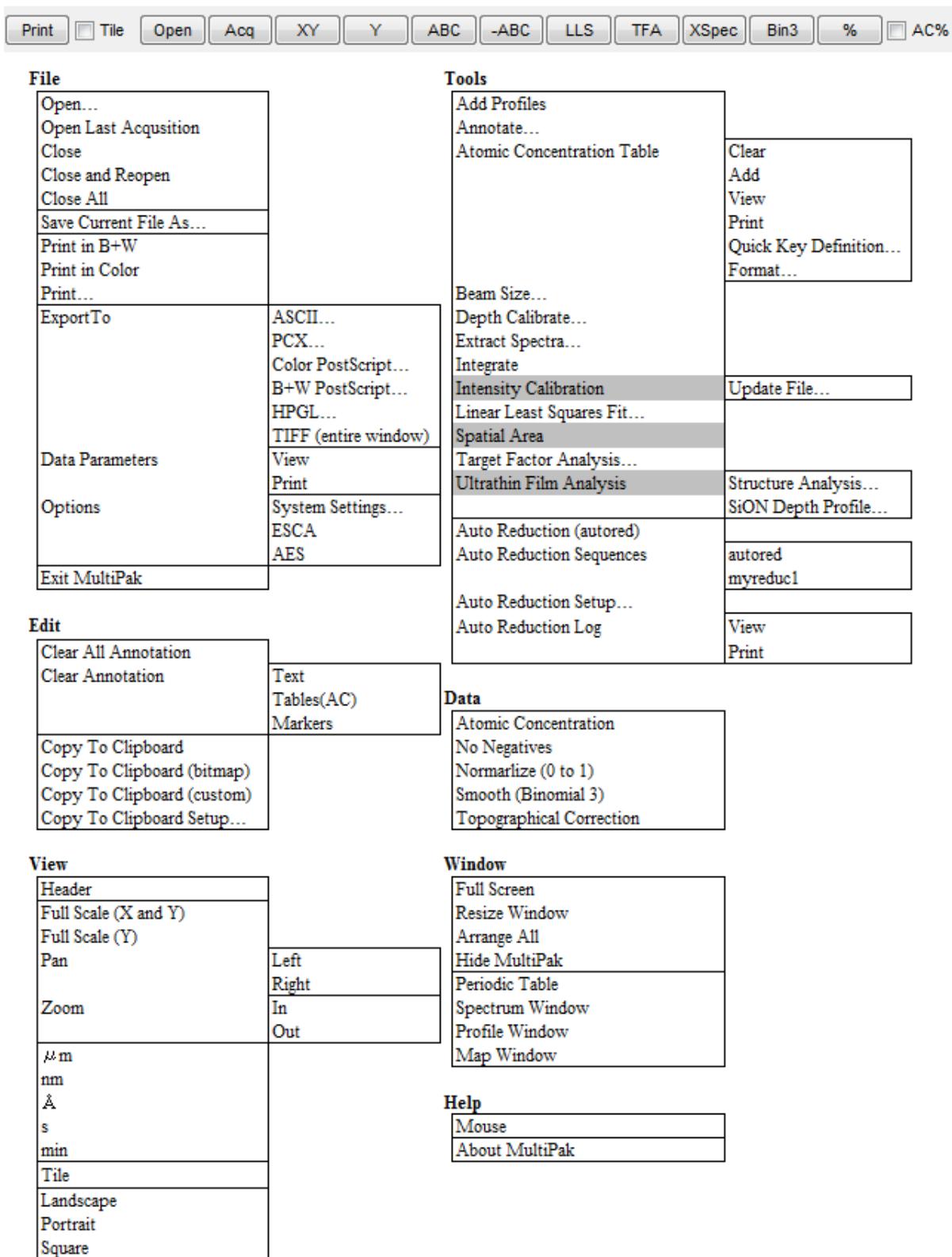


Figure 1-5. Menus and Upper Toolbar in the ESCA **Profile** Window.  
(The shaded functions are not available in the AES Profile window.)

## 1: Introduction and Overview

Table 1-3. Mouse Functions in the **Profile** Window.

To:	Point At:	Press:
Select/deselect profile (region)	region button in region bar	Left
Select subregion (created in LLS or XSpec by dragging left mouse button)	subregion boundary	Left
View lower and upper x (or y) coordinates of the subregion	subregion boundary	[Shift]-Left
Expand (zoom in to) horizontal, vertical, or diagonal subregion	anywhere within current x and y axes	Left & drag
Redraw boundaries of a region or subregion	region or subregion boundary	Left & drag
Move a region or subregion boundary	region or subregion boundary	Left & drag
Move region or subregion boundaries without changing the current range	region or subregion boundary	Right & drag
Automatically generate atomic concentration table	“%” (Atomic Concentration Table ‘Quick Key’) on the upper toolbar	Left
View and/or change axis titles and/or axis start and end points	x or y axis	[Shift]-Left
Change the arrangement of multiple displays	View–Landscape, –Portrait, or – Square	Left
Scroll left and right along the profile	View–Pan, or drag subregion cursor outside left or right axis	Left
Select units of measure of depth axis	□m, nm, Å, s, or min on the View menu	Left
Normalize all profiles for data comparison	Data–Normalize	Left
Perform linear least squares fit on data	Tools–Linear Least Squares Fit..., or LLS pushbutton on upper toolbar	Left *
Perform target factor analysis on data	Tools–Target Factor Analysis..., or TFA pushbutton on upper toolbar	Left *
Perform binomial smooth on data	Data–Smooth (Binomial 3), or Bin3 pushbutton on upper toolbar	Left
Correlate time data to depth data for redisplay	Tools–Depth Calibrate...	Left *
Extract spectra from profiles	XSpec on the upper toolbar; Spec/New or Spec/Upd on the lower toolbar; or Tools–Extract Spectra...	Left

\* Pressing this mouse button displays additional options. See the function in Section 3 for details.

## 1: Introduction and Overview

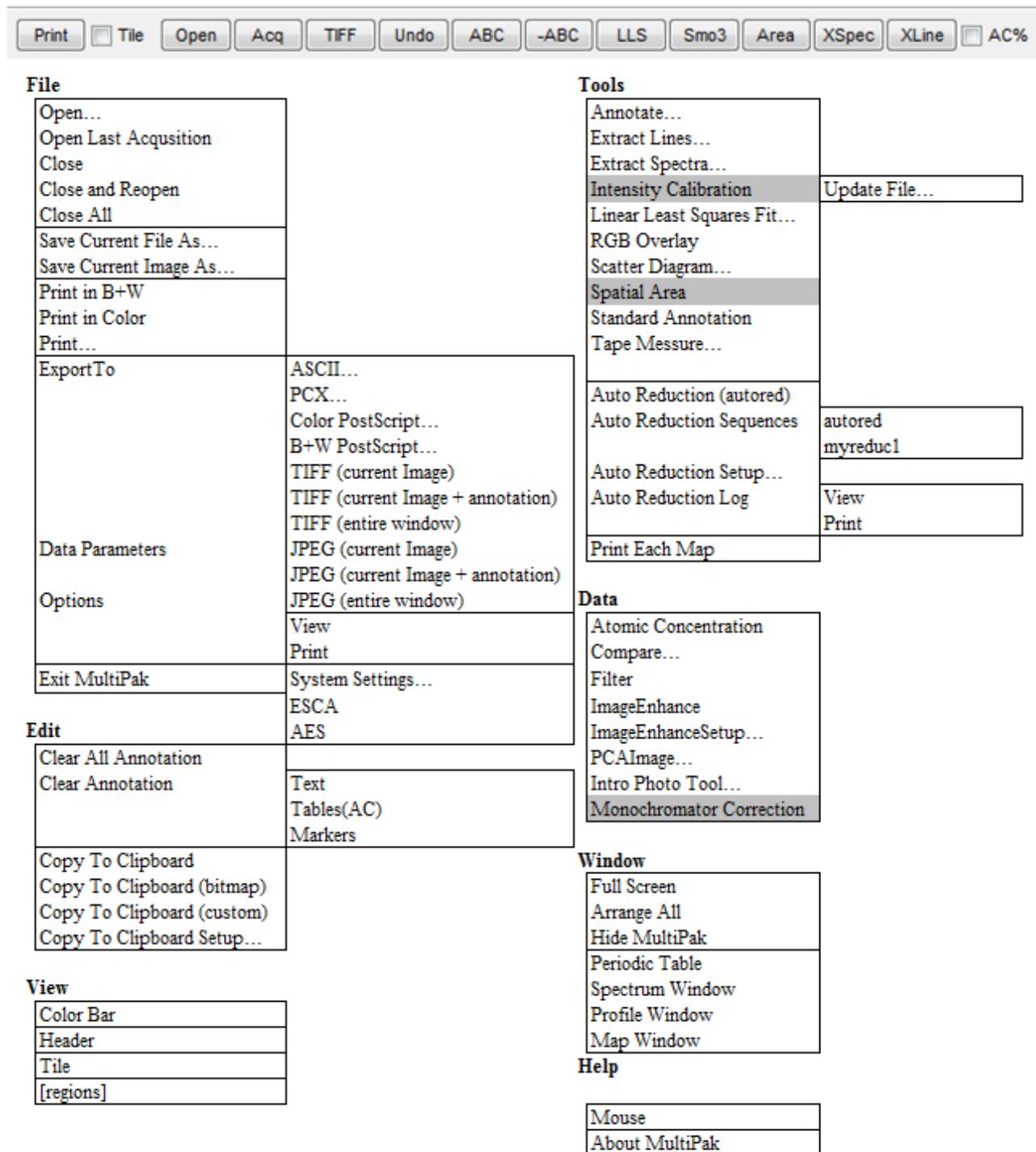


Figure 1-6. Menus and Upper Toolbar in the ESCA Map Window.  
(The shaded functions are not available in the AES Map window.)

## 1: Introduction and Overview

*Table 1-4. Mouse Functions in the Map Window.*

To:	Point At:	Press:
Select map (region)	map named for that region or checkbox for that region in lower toolbar or region name on View menu	Left
Select subregion (defined in LLS, XLine, or XSpec by dragging left mouse button)	subregion boundary	Left
View lower and upper x (or y) coordinates of the subregion	subregion boundary	[Shift]-Left
Display subregion spectra	Spec/Line New/Upd in lower toolbar	Left
Delete boundaries of a subregion	1. Subregion boundary 2. Cut button	1. Left 2. Left
Move a subregion boundary	anywhere within subregion boundaries	Left & drag
View and/or change lower and upper x coordinates of the subregion	subregion boundary	[Shift]-Left
Modify the display of the image	Data–Filter...	Left *
Divide the data in the image by the data in a reference image	Data–Compare...	Left *
Combine three color-coded images	Tools–RGB Overlay	Left *
Draw a measurement on the image	Tools–Tape Measure...	Left *

\* These functions have special mouse actions once the function has been activated. See Section 3.

## 1: Introduction and Overview

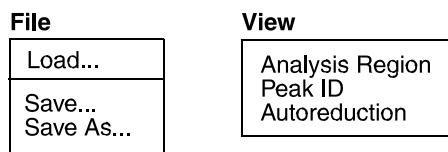


Figure 1-7. Menus and Option Menu in the **Periodic Table** Window.

Table 1-5. Mouse Functions in the **Periodic Table** Window.

To:	Point At:	Press:
Select (or deselect) an element	element abbreviation in periodic table	Left
Open Transition dialog box	element abbreviation in periodic table	[Shift]-left
Turn off all buttons in the periodic table	Clear button below periodic table	Left
Toggle the AES Fingerprint display on and off	element abbreviation in periodic table	Right

## Contacting ULVAC-PHI Customer Service

If any ULVAC-PHI -manufactured or -supported controls or equipment fail or other problem-solving is needed, contact ULVAC-PHI Customer Service as follows:

### **By mail:**

Copyright © 2010  
ULVAC-PHI, INC.  
370 Enzo, Chigasaki, Kanagawa,  
253-8522, Japan

### **By e-mail:**

service@phi.com

### **By telephone or fax:**

Region	Telephone	Fax
U.S.	1-952-828-6200	1-952-828-6176
Japan/Asia	81-46-785-6522	81-46-785-4411
Europe	49-89-96275-0	49-89-96275-50

### ***Reporting Software Performance Issues***

A template file called “mpspr.txt” was installed with MultiPak for the operator to report software issues. The file contains a form called “Software Performance Report.” Table 1-6 lists where the file is located and what operating system software to use to open the file. The procedure is as follows.

1. Open the text editing application installed with your computer’s operating system.
2. Open the file named “mpspr.txt.”
3. Complete the form, referring to the information in Table 1-7.

*NOTE: Please feel free to use the editing capabilities. For example, the business address need not be limited to a single line.*

4. Save the document using the Save As... function of the application software.

*NOTE: Using the Save As option will leave the original, empty template intact for later use.*

5. Mail, fax, or e-mail the performance report to ULVAC-PHI Customer Service.

## **1: Introduction and Overview**

*Table 1-6. Software Performance Report File.*

Computer	Directory	Application
PC	\multipak\v9.0\mpspr.txt	Notepad

*Table 1-7. Fields of the Software Performance Report.*

Field	Description
Company Name	Name of the business that owns the MultiPak software.
User Name	Name of the system operator or contact person.
Business Address	Mailing address for mail that may come from Physical Electronics. (Include internal mail-stop information.)
TEL	Telephone number of User. (Include area code and country code, if applicable.)
FAX	Complete telephone number to which to transmitting facsimiles.
MultiPak Version	Version of MultiPak with which the issue came up.
Model Number of System	Model number of the PHI system with which MultiPak is being used. (Example: Quantera, 700).
Analysis Techniques	Indicate "ESCA," "Auger," or both.
Description of Issue	A detailed account of the problem or concern. The goal is to provide ULVAC-PHI Customer Service with enough information so that ULVAC-PHI can recreate the occurrence. (Many issues are intermittent or depend on the events that led up to the occurrence.) Such details help ULVAC-PHI address the issue in a timely fashion.  <i>NOTE: A copy of the data file being used at the time of the occurrence should be sent along with the performance report.</i>

## Translating Data Files into MultiPak Format

Data acquired using PHI ACCESS, PC-ACCESS, COMPASS, *SpecView*, or PC-*EXPLORER* data acquisition software can be saved in or translated to MultiPak format. The appropriate function for each software package is listed in Table 1-8.

*Table 1-8. Data File Translation Functions.*

Software	OS	Function
PC-ACCESS	PC	At the DOS prompt, type: \phi\exe\phic^tpak^<filename> where <filename> is the complete path and file name.*
SpecView	PC	File–Data Conversion–Export–MultiPak Files
PC-EXPLORER	PC	File–Save As MultiPak
ACCESS	Apollo	At the OS prompt, type: phic^tpak^<filename> where <filename> is the complete Apollo name of the file.*
COMPASS	Sun OS	No translation necessary

"^" indicates that a space is typed.

## Downloading MultiPak Update Program File

The latest update will be available at the following ULVAC-PHI web site. A user id and registered password are necessary to download it. Regarding the update procedure, please refer the Update instruction document in the set of download files.

ULVAC-PHI Web Site :

<http://www.ulvac-phi.co.jp/>

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\* See Appendix D for information about transferring the translated files to a PC.



## **Section 2: Getting Started**

---

This section is intended to help new users get started with MultiPak. The topics included are the following:

- Installing MultiPak on a PC,
- Starting MultiPak,
- Analysis Data Set,
- File Locations,
- Getting Familiar with Windows,
- Installing Tutorial Files,
- PC Tutorial—Data Reduction of AES Data Files,
- PC Tutorial—Data Reduction of XPS Data Files.

### **Installing MultiPak on a PC**

*NOTE: Any previous version of MultiPak and older versions of the MCR (MATLAB Component Runtime) software should be uninstalled prior to installation of a new version of MultiPak. Uninstall the software using the Add or Remove Programs tool in the Windows Control Panel. If you have a newer version of the MCR that was previously installed with MultiPak Versions 8.2C or Version 9 it is not necessary to uninstall and reinstall the MCR and you can proceed to step 14 after uninstalling the previous version of MultiPak.*

*NOTE: If you have modified the Periodic Table databases and want to import these changes into the new version, you must make a backup copy the Periodic Table databases ‘aes.edb’ and ‘xps.eddb’ prior to uninstalling the old version of MultiPak. These databases are located at: ‘MultiPak\vxX\Userdata\Common\Database’ in the Multipak folder.*

The MCR (MATLAB Component Runtime) software must be installed prior to installing MultiPak.

1. Insert the MCR software compact disc (CD) into the CD drive of your computer.
2. Execute the file named MCRInstaller.exe if the installation does not start automatically.
3. At the Select language prompt, select[English] and click on [OK]

## **2: Getting Started**

4. The next window will prompt you to install VCREDIST\_X86, click on the [Install] button to start installation.
5. At the MATLAB Welcome window, click [Next] to continue the software installation.
6. In the Customer Information window, enter a User Name and Organization information, then click [Next].
7. In the Destination Folder window click [Next].
8. In the Ready to Install Program window click on [Install] to start the MCR software installation.
9. When the MATLAB InstallShield Wizard Completed window appears, click on [Finish], the installation of MCR software is finished. Leave the MCR disk in the CD drive.
10. Select My Computer on the computer desktop and select the CD drive. Double click on the Vcredist2008 folder and execute the file named vcredist\_86.exe. Note: if this software has been previously installed a Maintenance Mode window will appear. If this appears you can select [Cancel] or [Repair]. Repair will reinstall the Vcredist2008 software.
11. In the Microsoft Visual C++2008 window, click on [Next] to start the installation.
12. In the license Terms window, check [I have read and accept the license terms.] check-box. And then click on [Install] to continue the installation.
13. When the Setup Complete window appears, click on [Finish], the installation of Vcredist\_x86.exe is complete.
14. Next, Install the MultiPak software. Insert the MultiPak software compact disc (CD) into the CD drive of your computer.
15. Execute the file named SETUP.EXE if the installation does not start automatically.
16. In the Welcome to the InstallShield Wizard for MultiPak 9.0 window, click [Next] to continue the software installation.
17. In the Customer Information window, enter a User Name, Organization information, and the Password key located on the back of CD case. Then at the Install this application for: prompt select Anyone who uses this computer and click [Next] to continue the installation.

18. In the Setup Type window, select Typical to install the full version:

- Note: Typical and will install the full version of MultiPak, which includes: the MATLAB server, MultiPak, the AES Handbook data, the XPS Handbook data and the Tutorial data.
- Note: Custom will give you the options to select which data libraries will be installed.

19. In the Ready to Install the Program window, click on [Install] to start the software installation.

20. When the Installshield Wizard Completed window appears, click on [Finish]. MultiPak installation is now complete. It is recommended that you Restart the computer before using MultiPak.

## Starting MultiPak

To start MultiPak, double-click on the MultiPak icon on the Windows desktop or select PHI-MultiPak from the Start menu.

If MultiPak has already been started, open MultiPak by clicking on the MultiPak button in the windows tool bar at the bottom of the screen or by clicking on the Show MultiPak icon on the Windows desktop.

## Analysis Data Set

MultiPak analyzes data acquired using Physical Electronics surface analysis instrumentation for X-ray Photoelectron Spectroscopy (XPS) or Auger Electron Spectroscopy (AES). This subsection briefly describes the types of files that can comprise an XPS or AES data sets and other general information about a data sets that a MultiPak user should be aware of.

### ***File Types for AES or XPS Data Sets***

AES or XPS data can include some or all of the following types of files:

- Spectra, stored in files having the extension “.SPE,” which will open in the MultiPak Spectrum window. Each file contains a series of data points, in the E N(E) format, from one point (stationary electron beam was positioned on a specific point) or area (rapidly scanned or rastered over an area of the surface). Spectra are acquired either as surveys or multiplexes. A *survey* is a quick scan over a wide contiguous energy range to survey the elements present in a sample. A *Multiplex* is a high-resolution scan of several narrow energy ranges to obtain enhanced sensitivity and spectral detail.
- Maps, stored in files having the extension “.MAP,” which will open in the MultiPak Map window. Maps provide information on the two-

dimensional surface distribution of an element across the selected analysis area.

- Line scans, stored in files having the extension “.LIN,” which will open in the MultiPak Profile window. Line scans provide information on the surface distribution of an element along a straight line through the selected analysis area.
- Depth profiles, stored in files having the extension “.PRO,” which will open in the MultiPak Profile window. Profiles provide information about the distribution of an element as a function of depth by a combination of collecting spectra and sputtering to remove material.
- In addition to element Maps, secondary electron, and optical images can be opened in the MultiPak Map window. These images are typically used to define analysis points or areas. For some instrument types these images are linked to data files and the location of the analysis point for a specific data file can be displayed on the image in MultiPak. These image file types are as follows:
  - AES images stored in files having the extension “.SEM” (scanning electron micrograph image), “.BSE” (backscattered electron image), and/or “.ABS” (absorbed current image);
  - XPS images stored in files having the extension “.SXI” (secondary electron x-ray induced image) and/or “.PHO” (digital optical photograph).

### ***Other Important Information Stored with Data Files***

In addition to the spectral data contained in data files, important information about how and where the data file was collected is stored with the data file. This information may include: location on the sample, sample tilt angle, excitation energy, neutralization conditions, etc. Some of this information is displayed in the MultiPak data header and additional information is available by Viewing the Files Data Parameters.

## **Handbook Data Files**

Spectra from the PHI Auger and XPS Handbooks are stored in the following locations:

AES Handbook data: C:\multipak\datafile\handbook\aes

ESCA/XPS Handbook data: C:\multipak\datafile\handbook\esca

## **Tutorial Files**

MultiPak is installed with the following sample data files:

- **AES:** *AESSPEC.SPE, TINTI.PRO, LINEWINDOW.LIN, 5KXSEM.SEM,* and *AUGERMAP.MAP*;
- **ESCA:** *PET.SPE, XPSPROF.PRO, TONER.MAP*, and *TONER.SXI*.

These files are to be used with the tutorials contained in the remainder of this section. Note that many of the illustrations in this manual were created using these data files.

## PC Tutorial—AES Data Reduction

This section describes how to use the software tools in MultiPak that are commonly applied to analyze (reduce) AES spectra, maps, and sputter depth profiles.

### **Analyzing an AES Spectrum**

A survey spectrum is typically a quick, high-sensitivity acquisition of Auger data over a wide energy range. A survey spectrum is commonly used to identify which elements are present in the selected analysis area. The typical data reduction procedure involves differentiating the data, identifying the peaks, labeling the peaks, obtaining atomic concentration data, and outputting the results. Element identification is demonstrated both manually and using the Peak ID function.

1. Open the AES spectrum file, as follows:

- a. Locate the Tutorial data folder :

File\Open\Browse\ c:\Multipak\Datfile\Tutorialdata\AES

- b. Select File—Open. The Open dialog box is displayed.

- c. Select .SPE or \*.\* in the File Type field, then double-click on AESSPEC.SPE (or click on the file name so it becomes highlighted, then click on OK).

The survey spectrum is displayed in the MultiPak Spectrum window. Notice that the file's name is displayed in green, indicating that this data is "selected." Any MultiPak functions activated will be applied to this data.

The file header (displayed only when Header in the View menu is checked) lists the file's data acquisition parameters (date of acquisition, beam voltage of acquisition, etc.)

2. Auger spectra are typically differentiated to remove the rapidly changing background and make it easier to observe the Auger peaks. Survey spectra are most often collected with 1 eV data step sizes and for this reason 5, 7, or 9 point differentiation is commonly applied.

- a. Select Data—Smooth/Derivative Setup.... The function options are displayed in the lower toolbar.

- b. Check the "Derivat" check box to turn the derivative function on.

- c. In the "Derivat," pull down menu select "5."

d. Turn the “SavGol” radio button on. A black dot should appear in the center of the radio button. This turns the Savitsky-Golay smoothing function on and the Binomial smoothing function off.

e. In the “SavGol,” pull down menu select “5.”

Note: The smooth/derivative button in the upper toolbar has been named “S5D5,” so that the next 5-point differentiation and 5-point smooth can be performed by simply clicking on the S5D5 button without having to open the Smooth/Derivative Setup menu.)

f. Click on the Filter button in the lower toolbar. The smoothed and differentiated data will be displayed in the Spectrum window.

g. Click on the Exit button in the lower toolbar. This closes the Smooth/Derivative Setup menu.

*NOTE: The processing history during this session on AESSPEC.SPE is given on the third line of the data file header. In this case “S5D5”.*

3. Identify the Auger peaks *manually* using the Energy Cursor function, as follows:

a. Energy cursor setup:

Select File–Options–Energy Cursor. Its submenu is displayed. Click on “Selected Elements.” This will only display labels for elements that have major peaks in the Energy Cursor database when step ‘b’ is performed.

Note: If All Elements is selected, *all* elements in the Energy Cursor database for that energy will be shown.)

b. Find and annotate each peak as follows.

Then, click and hold down the right mouse button inside the axes of the spectrum data, drag the vertical cursor until it is aligned with the lowest point of the largest peak on the data curve, and release the mouse button. The annotation is displayed rotated 270 degrees.

If you wish to expand the display around a specific peak, click the left mouse button to the left of a peak, then drag the cursor to the right side of the peak and release the button. The display will change to show an “expansion” of the data that was highlighted during the click and drag. (The expansion can be undone by pressing the XY button in the upper toolbar.)

## 2: Getting Started

The major peaks in this spectrum and the annotation generated are:

–	~ 80 eV	Hg, Tl, U
–	~ 269 eV	C, Ru
–	~ 510 eV	O, I
–	~ 1615 eV	Si, Hf

- c. If you wish to change the display of peak labels or other text, click on the ABC button in the upper toolbar, which displays the Annotate menu in the lower toolbar. Select Peak as the annotation type, and select 0 for rotation. Press the Apply All button. Press Exit. The result will look similar to Figure 2-1a.
- d. Using the *Handbook of Auger Electron Spectroscopy*, compare the peaks in the acquired data to the standard spectra for each of the possible elements to make a positive identification of the element for which this is a peak.\*

The correct identifications of these peaks are Si (in the oxidized state\*) at ~80 eV, C (carbon) at ~269 eV, O (oxygen) at ~510 eV, and Si (silicon) at ~1615 eV, as illustrated in Figure 2-1b.

4. Identify the element peaks *automatically* using the Peak ID function, as follows:
  - a. Press the –ABC button (or select Edit–Clear All Annotation) to clear all existing annotation.
  - b. Select the “Element Labels” mode: In the options pull down in the lower portion of the Periodic Table window select “Element Labels”.
  - c. In the Spectrum window, press the ID button in the upper toolbar.

The peak labels Si, C, and O are added to the spectrum display. The corresponding element region buttons are displayed in the Spectrum window’s region bar, and the corresponding buttons are turned on in the Periodic Table window.\*\* If View–Region Cursors is on, the region boundaries are also displayed. The result will look like Figure 2-2.

*NOTE: Pressing one of the region buttons in the region bar of the*

---

\* Refer to the procedure in Section G.1 on page 20 of the handbook.

\* See page 14 of the handbook.

\*\* Si2, C1, and O1 are the Auger “transitions” of the most intense peaks in the standard spectrum of each of these four elements.

## **2: Getting Started**

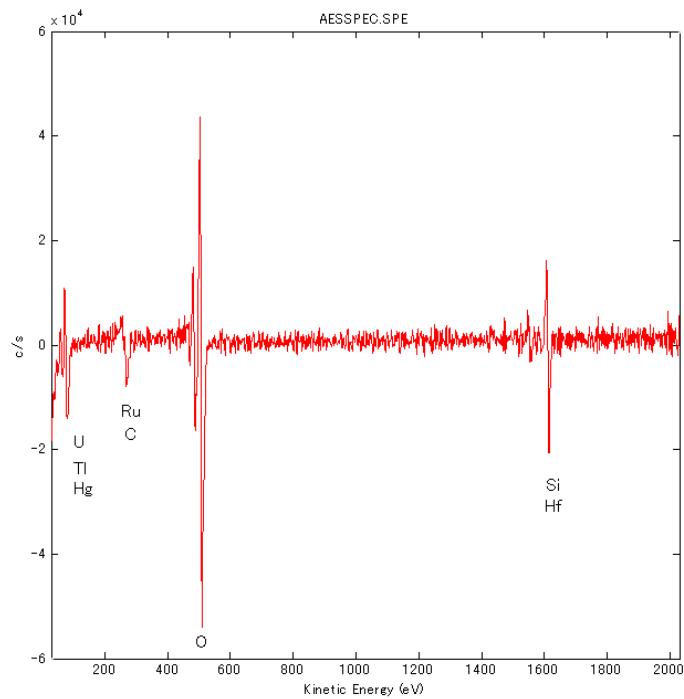
*Spectrum window automatically “expands” the display to the defined region for the peak. Pressing one of the activated element buttons in the Periodic Table removes the region button and the region’s boundaries from the data displayed in the Spectrum window.*

*NOTE: The Peak Identification function does a better job of identifying peaks correctly than does Energy Cursor, because Peak Identification compares spectra, not just individual energies. For example, silicon is identified by the Peak Identification routine whereas mercury is not, because both major peaks of silicon oxide are recognized but only one of the Hg peaks is detected.)*

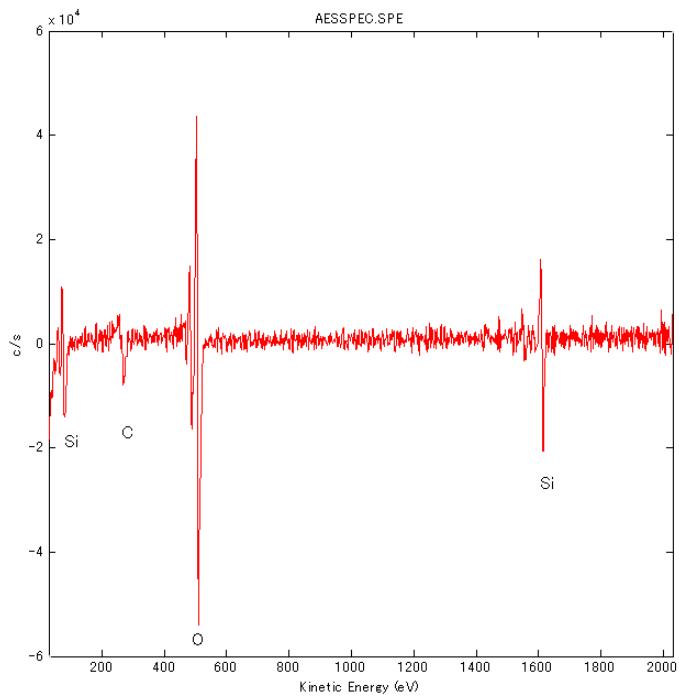
5. Multiple options are available to output the processed spectrum:
  - a. Print directly from MultiPak by pressing Print in the upper toolbar (or selecting File–Print in B+W or Color).
  - b. Paste the processed spectrum into another application as follows:
    - Select Edit–Copy To Clipboard.
    - Open the application on the desktop and select the Paste function, which is how Figure 2-3 was added to this document.
  - c. Export the spectrum display to a graphics file, as follows:
    - Select File–Export To–PCX....

A file with a PCX extension, like that shown in Figure 2-3, is created and placed in a MultiPak subdirectory (default is c:\multipak\datafiles\phi1user1\aes).

## 2: Getting Started



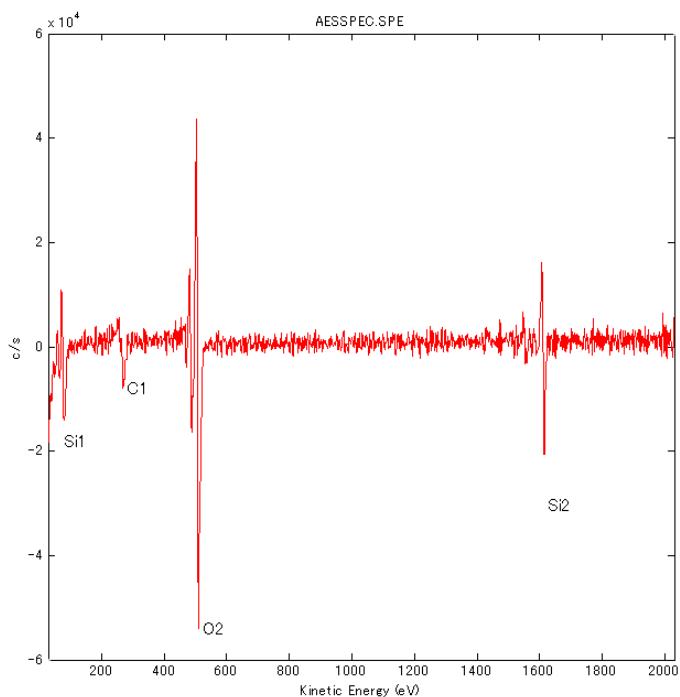
a. Result of Energy Cursor Function.



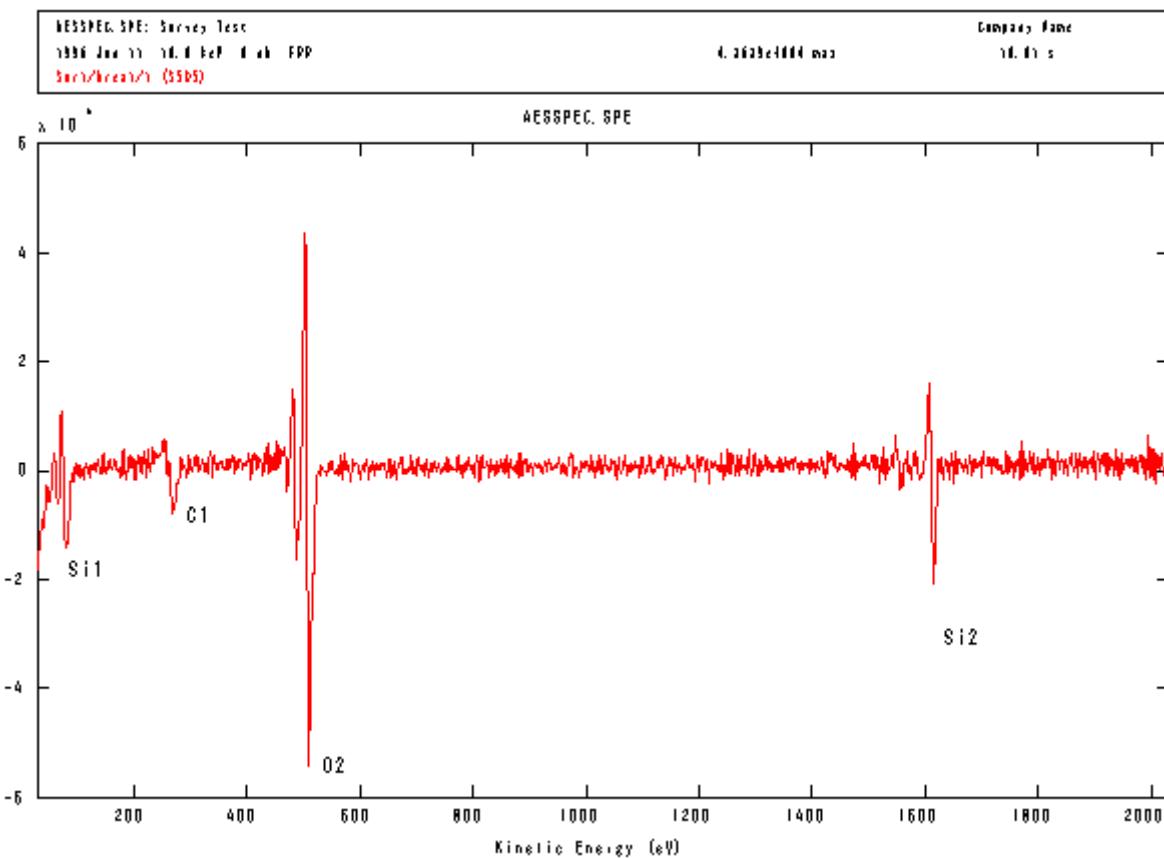
b. Result after Operator's Analysis and Removal of Some Peaks.

Figure 2-1. Peak Identification by Operator Using Energy Cursor.

## **2: Getting Started**



*Figure 2-2 Result of Automatic Peak Identification after Rotation.*



*Figure 2-3. PCX File of the Data Shown in Figure 2-2.*

## 2: Getting Started

6. Generate an atomic concentration table, as follows:
  - a. Any previous annotation or AC tables can be removed from the display by clicking on them and dragging them off the display.
  - b. Press the % button in the upper toolbar (or select Tools–Atomic Concentration Table–Add, then Tools–Atomic Concentration Table–View).

The relative atomic concentrations are calculated for the regions present in the region bar. The Notepad application opens to show the table, as shown in Figure 2-4).

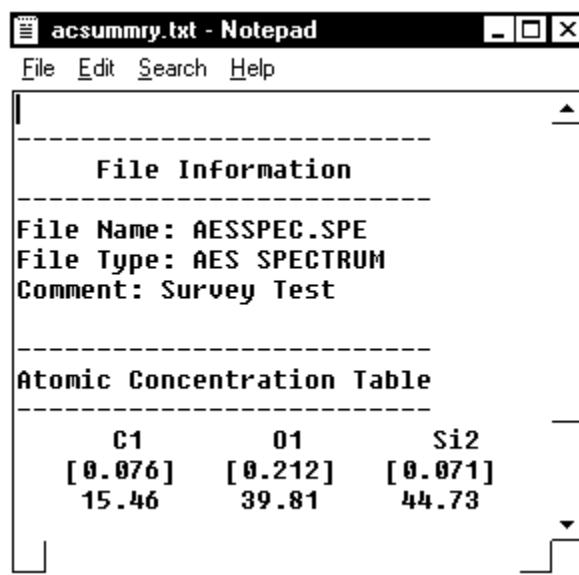


Figure 2-4. Atomic Concentration Table from AESSPEC.SPE.<sup>1</sup>

7. Output the AC table in different ways, as follows:
  - a. Print directly from Notepad:
    - In the Notepad window, select File–Page Setup..., Printer... to designate where the table will be printed.
    - Select Print in B+W.
  - b. Save the table as a text file, as follows:
    - In the Notepad window, select File–Save As....
    - Enter a file name and destination directory, and press OK.

---

<sup>1</sup> The format of the AC table is determined by the settings in the AC Table Setup dialog box. The numbers in brackets below the transition names are the sensitivity factors used in the calculations.

- c. Paste the table into another text file, as follows:
    - In the Notepad window, select Edit–Copy.
    - Open another text application on the desktop and select the Paste function (usually under the Edit menu). The table is pasted into the document.
  - d. Close the Note Pad application
  - e. Use the %ABC button in the upper tool bar to place a simple AC table on the spectrum display. The table can be repositioned by clicking and dragging it.
8. Select File–Close from the Spectrum window menu.

### ***Analyzing an AES Depth Profile***

Auger depth profiles provide compositional data as a function of depth. The following sequence examines the acquired data for peak shape changes as a function of depth and uses linear least squares (LLS) fitting to extract different chemical states of the measured elements.

1. Turn on the Data Link check boxes in both the Spectrum window's and Profile window's lower toolbar, if they are not on already.
2. Open the AES profile data file, as follows:
  - a. Select File–Open. The Open dialog box is displayed.
  - b. Select .PRO or \*.\* in the File Type field, then double-click on TINTI.PRO (or click on the file name so it becomes highlighted, then click on OK).

The file opens in the Profile window, and the Spectrum window displays all the spectra used to create the profile.

3. Perform a 5-point differentiation on the spectral data, as follows:

*NOTE: Differentiation and smoothing have the potential to remove spectral fine structure if applied to heavily. For this reason we recommend using 5, 7, or 9 point smoothing and differentiation.*

- a. In the Spectrum window, select Data–Smooth/Derivative Setup....
- b. In the lower toolbar, turn the Derivat check box on, and turn the SavGol and Binom buttons off.

## **2: Getting Started**

- c. Select 5 from the “Derivat.” pull down menu.
- d. Press Filter, and then Exit. The differentiated data is displayed.
4. In the region bar, turn on the N1 check box. The display changes to show only the data within the acquisition region boundaries of the N1 transition.
5. Drag the left, then right analysis region boundary (vertical cursor) toward the middle somewhat to remove possible end effects in the differentiated data.

Because LLS will be applied, only the edge effects should be taken out of the analysis region, retaining as much of the *structure* of the data inside the boundaries as possible. (If only peak-to-peak height were to be measured, the analysis region boundaries could be moved very close to the most positive and most negative excursions of the Auger peaks.)

6. In the Spectrum window, examine the spectra for the region, as follows:
  - a. Select the Select Spectra... function from the Tools menu of the Spectrum window. A selection bar with two colored horizontal lines is displayed to the right of the spectrum window.
  - b. Press the Show One button in the lower toolbar. The two colored horizontal lines appear as one line at the bottom of the selection bar.
  - c. Using the left mouse button, drag the colored line in the selection slider from the bottom to the top of the selection bar to observe how the peak shape changes with depth.
  - d. Press Show All in the lower toolbar to restore the display of all spectra.
  - e. Press Exit to leave the select spectra tool.
7. Repeat steps 4 through 7 for the regions Ti2, O1, and C1.

Since examination of the C1 region shows carbon at a low level in a single chemical state throughout the profile, an LLS fit on C is not performed.

8. In the Profile window, perform an LLS fit on nitrogen and titanium, as follows:
  - a. Press the LLS button in the upper toolbar.
  - b. Click, drag, and release the left mouse button in the data to create a

## 2: Getting Started

subregion like the one shown on the left side of Figure 2-5. Then, repeat to create a subregion like the one shown on the right side of the figure. The sub regions represent subsets of spectra with similar chemistry.

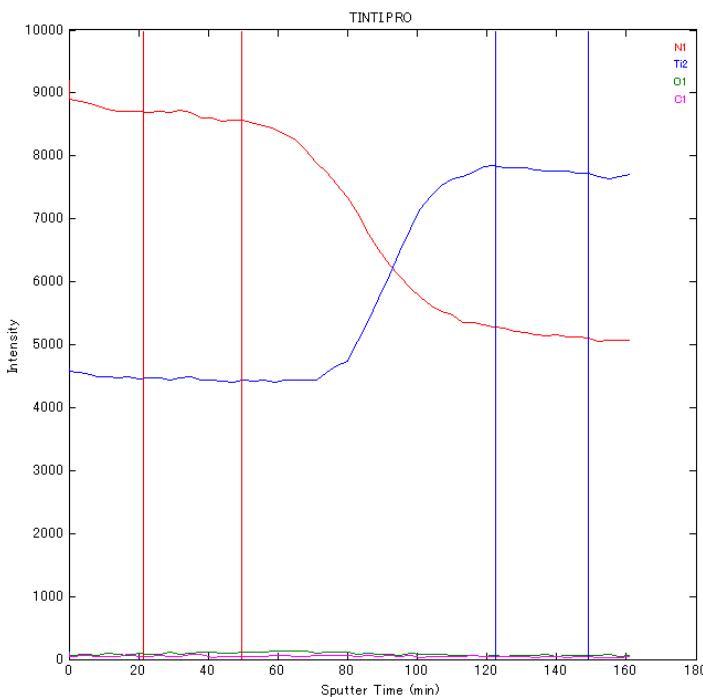


Figure 2-5. Two Analysis Subregions in the LLS Routine.

- c. Click on the N1 label in the upper right corner of the axes (or click on the curve displayed in the same color as the N1 label) to select the N1 curve.
- d. Press the Fit button in the lower toolbar. Figure 2-6 shows the result in the Profile window. Note: in version 9 and later it is not necessary to press the Fit button, fitting occurs automatically.
- e. Press the Spec/New button in the lower toolbar, then turn on the Data Link check box, if it is not on already. Figure 2-7 shows the composite spectra for the selected regions in the Spectrum window.

The left analysis subregion corresponds to TiN in the profile. Its associated curve in the Spectrum window is displayed in the same color as the subregion boundaries shown in the Profile window. This curve in the Spectrum window shows the overlapping peaks of the low-energy Ti LMM transition and the N KLL transition.

The right analysis subregion corresponds to Ti in the profile. This curve in the Spectrum window (in the same color as the right analysis subregion boundaries) shows the low-energy Ti LMM transition for elemental titanium.

## 2: Getting Started

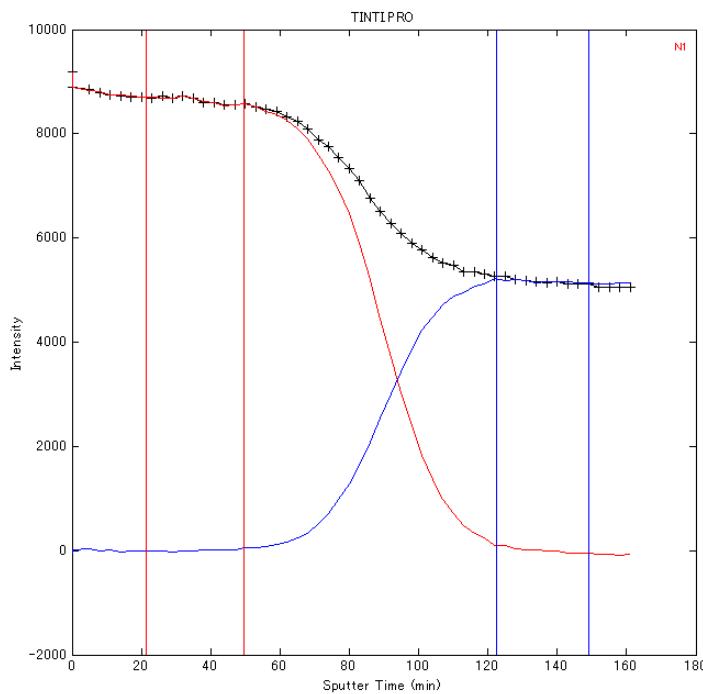


Figure 2-6. Result of the N1 Fit in the Profile Window.

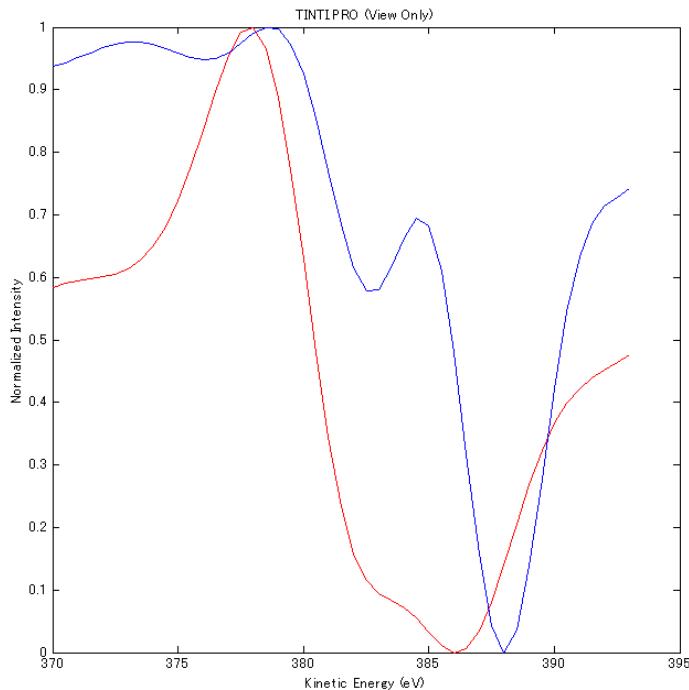


Figure 2-7. Composite N1 spectra from the selected regions shown in the Spectrum Window.

- f. Press the DispAll button in the lower toolbar to restore all the profiles to the Profile window including the LLS fitting results.
- g. Click on the Ti2 label in the upper right corner of the axes (or click on

the curve displayed in the same color as the Ti2 label) to select the Ti2 curve.

h. LLS fitting based on the shape of the composite spectra from the selected regions will automatically occur.

Figure 2-8 shows the result in the Profile window, and Figure 2-9 shows the composite spectra in the Spectrum window.

The left analysis subregion curve in the Spectrum window shows the high-energy Ti LMM transition in TiN, and the right analysis curve shows the high-energy Ti LMM transition in elemental titanium.

10. Select the oxygen profile, turn off the two subregions, and create a third subregion for oxygen:

- a. Press the DispAll button in the lower toolbar, then click on the O1 label (or the curve displayed in the same color as the O1 label).
- b. Click with the right mouse button on one of the subregion boundaries. The boundaries change from solid lines to dashed lines, indicating the subregion is currently not selected (active). Repeat this for the second subregion.
- c. Click, drag, and release the left mouse button to create one wide subregion that includes much of the data (Figure 2-10).
- d. The LLS fitting result for O1 will be displayed automatically.

The resulting LLS Fit result will have better a better signal to noise ratio than the original peak-to-peak data.

11. Press the Exit button in the LLS toolbar in the Profile window.

Five new “regions”—N1.ls1, N1.ls2, Ti2.ls3, Ti2.ls4, and O1.ls5—are added, as shown in Figure 2-11.

12. Turn off the following check boxes in the region bar to remove those curves from the display: Ti2, O1, C1, Ti2.ls3, Ti2.ls4, and O1.ls5.
13. If any of the three curves is displayed in the same color as another curve, [Shift]-left click on that curve to display the Data Properties dialog box. Select another color from the color option menu, and press Apply and Ok to change the color and exit the Properties dialog box.

## 2: Getting Started

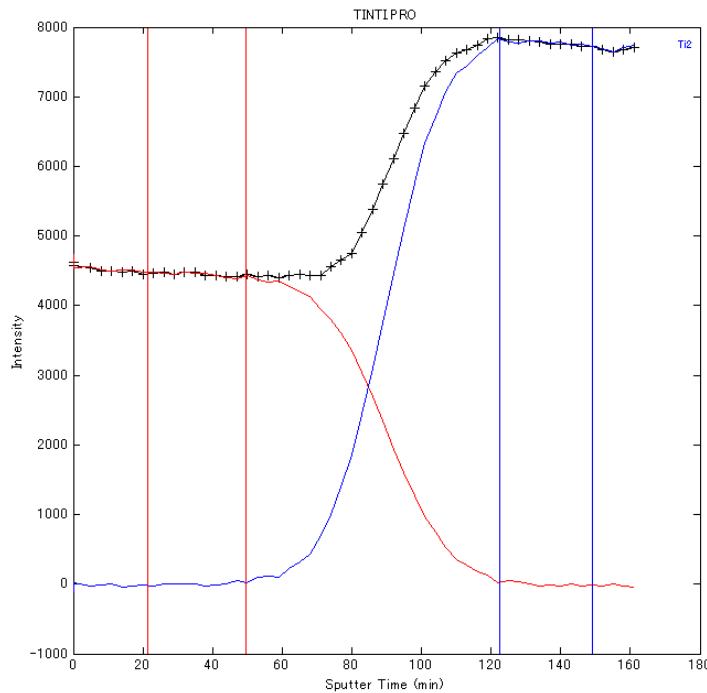


Figure 2-8. Result of the Ti2 Fit in the Profile Window.

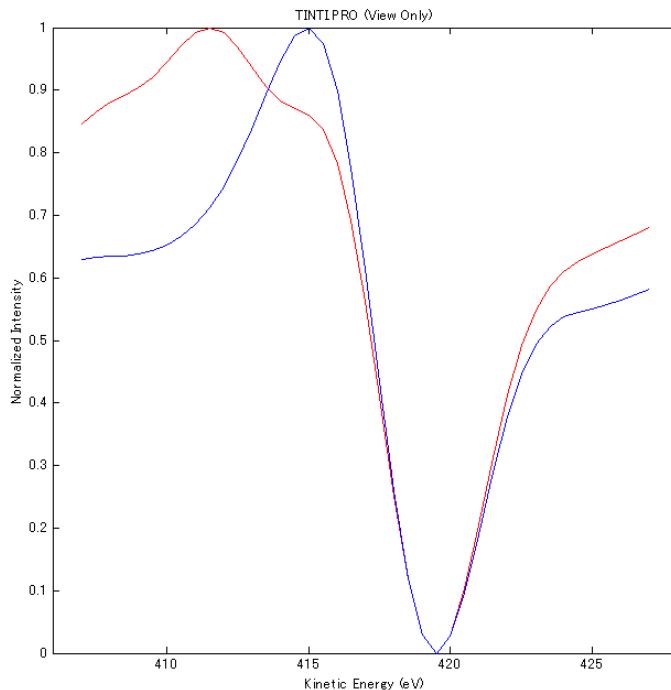


Figure 2-9. Composite Ti2 spectra from the selected regions shown in the Spectrum Window.

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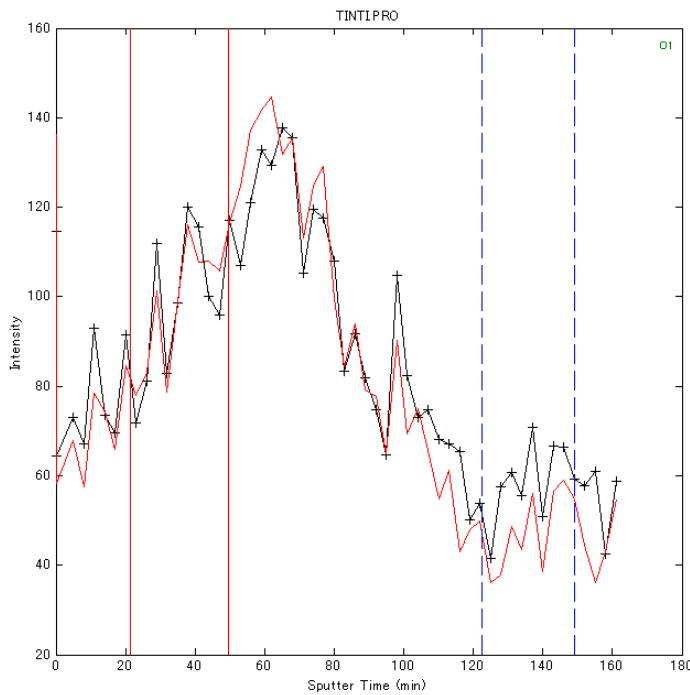


Figure 2-10. O1 Analysis Region during LLS Fit in the Profile Window.

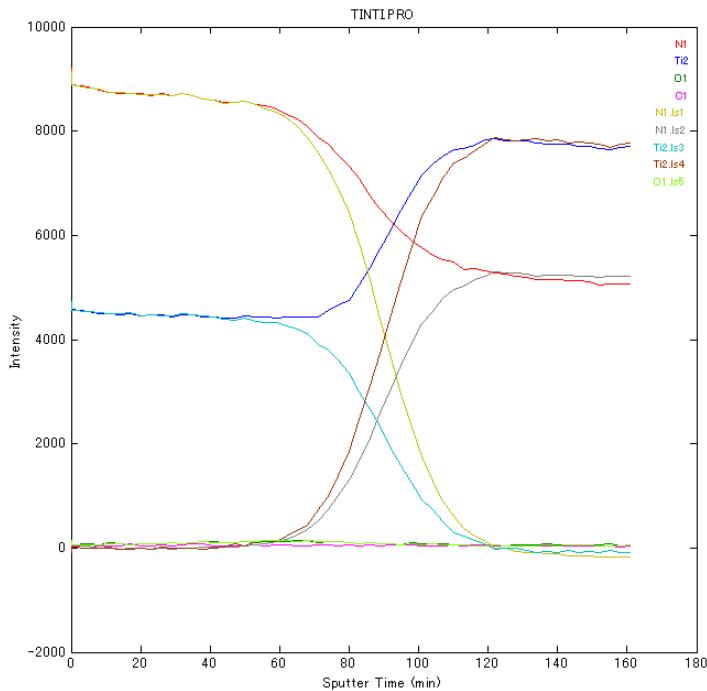


Figure 2-11. TINTI.PRO with the Five New Curves Created Using LLS.

14. [Shift]-left click on the x or y axis to display the Axis Properties dialog box. Change the Intensity minimum to zero to eliminate negative values from the display, and change the Time maximum to 170. Press Apply, then Exit.

## **2: Getting Started**

Figures 2-12 and 2-13 show the Axis Properties dialog box before and after eliminating the negative values from the display.

*NOTE: Selecting the No Negatives function from the Data menu is an alternative method to remove all negative values from the data set until a Close and ReOpen is performed on the data file. It is often preferable to simply eliminate them from the display.*

15. Annotate the data displayed, as follows:

a. Press the ABC button in the upper toolbar.

*NOTE: The user may also add text by clicking on a blank area within the axes and typing, without starting the Annotate function. This “free-form” annotation capability is also available during most MultiPak functions.*

b. Select Text as the annotation type in the lower toolbar.

c. In the color option menu in the Annotate toolbar, select the color of the TiN curve. Set rotation to 0, if it is not already. Select 11 in the font size option menu, click inside the axes, and type “TiN.”

d. In the color option menu in the Annotate toolbar, select the color of the Ti curve, click inside the axes, and type “Ti.”

e. In the color option menu in the Annotate toolbar, select the color of the original N1 curve, click inside the axes, and type “Original N1 Curve.”

f. In the color option menu in the Annotate toolbar, select white, click inside the axes, and type “Two chemical components extracted from N1 profile,” as shown in Figure 2-14.

g. Press Exit in the lower toolbar to close the annotation function.

16. Turn on the following check boxes in the region bar and turn off the other region buttons: Ti2, Ti2.ls3, and Ti2.ls4. Perform steps 13 and 14. Annotate the data displayed as shown in Figure 2-15.

17. Turn on the following check boxes in the region bar and turn off the other region buttons: Ti2.ls3, Ti2.ls4, and O1.ls5. Perform steps 13 and 14. Then, [Shift]-left on the O1.ls5 curve to display the Data Properties dialog box, type “10” in the Scale Factor field, and press OK (Figure 2-16). Annotate the data displayed as shown in Figure 2-17.

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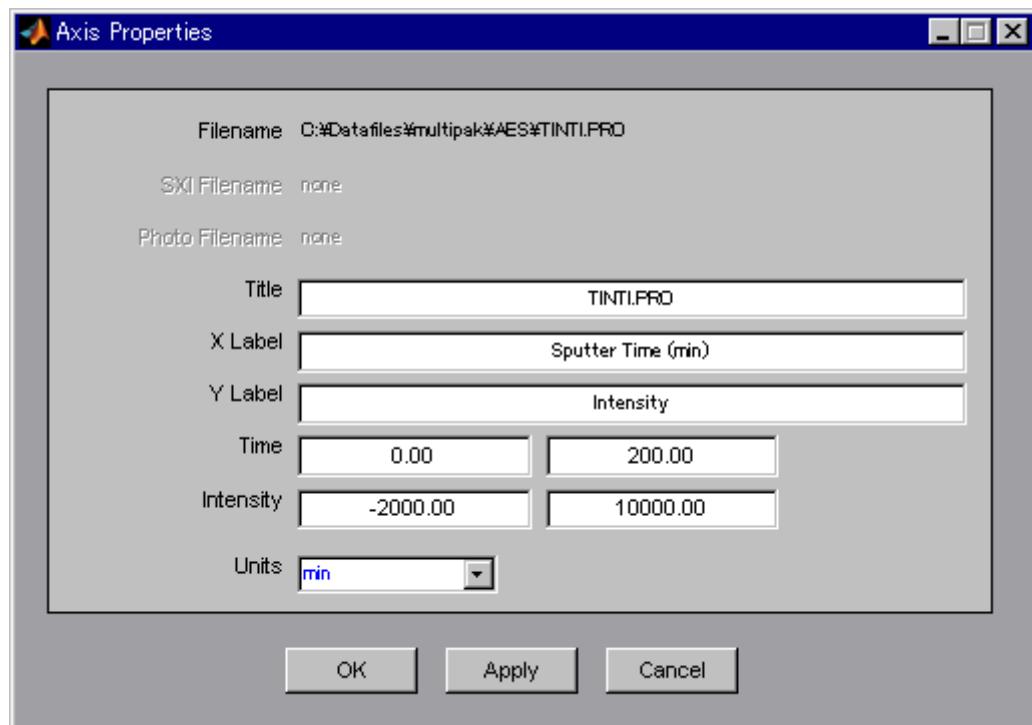


Figure 2-12. Axis Properties Dialog Box before Changing the Ranges of the X and Y Axes.

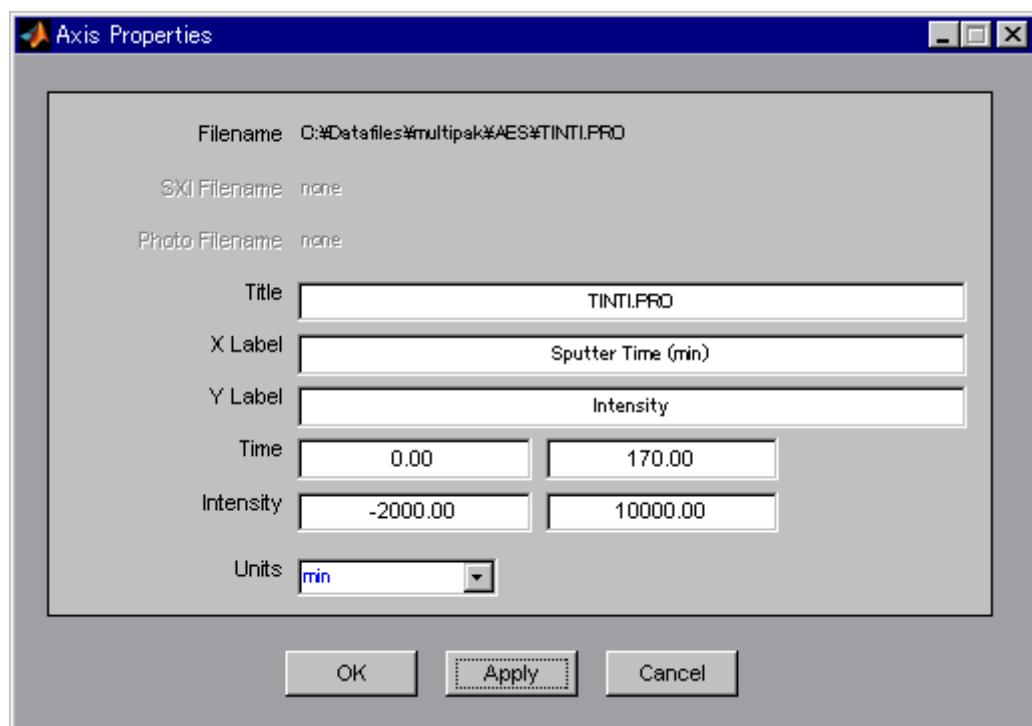


Figure 2-13. Axis Properties Dialog Box after Changing the Ranges of the X and Y Axes.

## 2: Getting Started

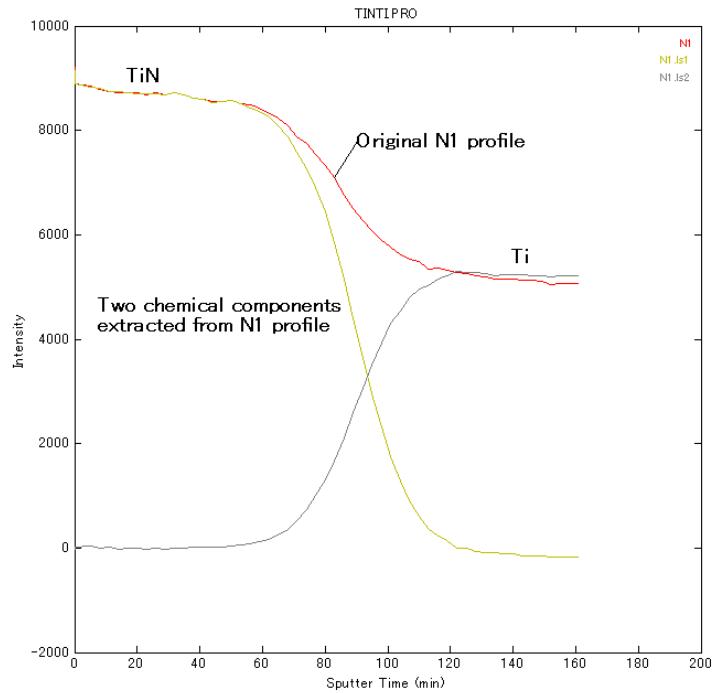


Figure 2-14. Annotated Nitrogen Curves.

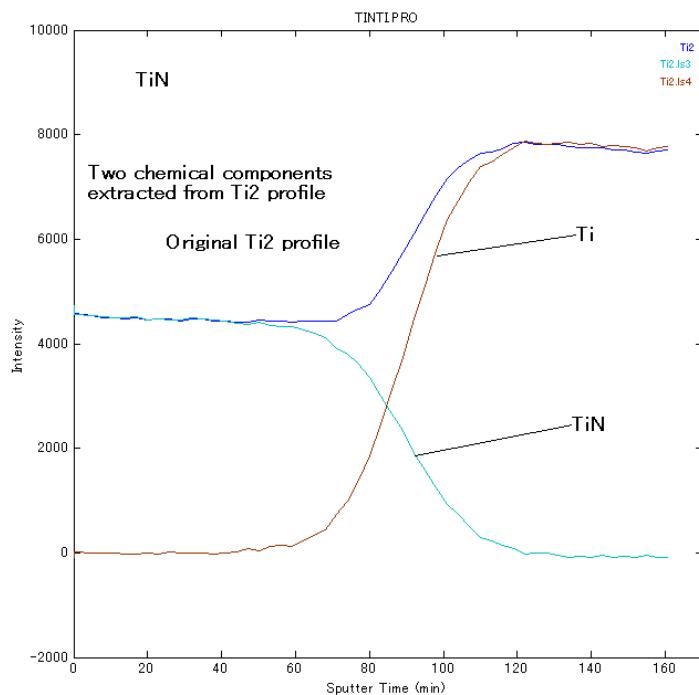


Figure 2-15. Annotated Titanium Curves.

## 2: Getting Started

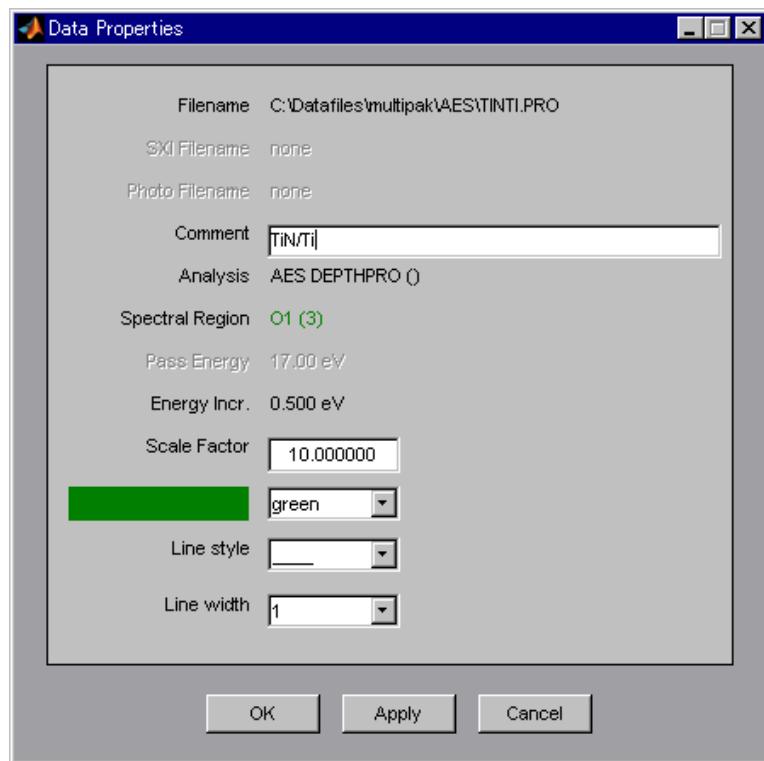


Figure 2-16. Scaling the Oxygen Using the Data Properties Dialog Box.

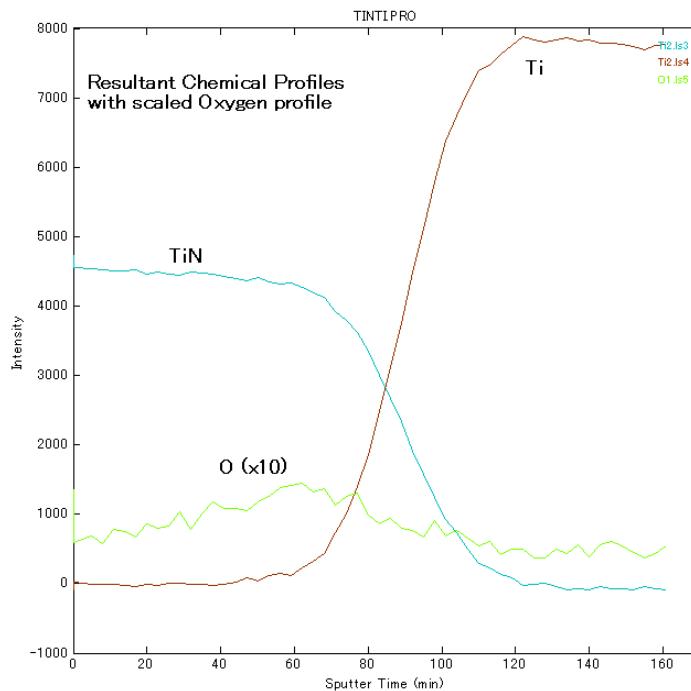


Figure 2-17. Annotated Titanium Curves with a Scaled Oxygen Curve.

### **Analyzing an AES Map**

An overlay of AES colorized maps provides a picture of the two-dimensional distribution of surface elements. Superimposing maps upon each other also can reveal unidentified areas on the surface.

1. Open the AES map file, as follows:
  - a. Select File—Open. The Open dialog box is displayed.
  - b. Select .MAP or \*.\* in the File Type field, then double-click on AUGERMAP.MAP (or click on the file name so it becomes highlighted, then click on OK).

The Map window opens and displays maps for the three element (Si, Au, & Ta) regions in the file. The maps will be displayed in the color mode that the color option menu is set to in the lower toolbar as shown in Figure 2-18.

To the right of the map of each region is the “color bar,” which has three sliding handles in the shape of arrowheads. The handle on the left can be dragged with the mouse to change the *brightness* of the displayed image. The two handles on the right can be dragged up and down, then to adjust the *contrast of the image*. After adjusting the contrast handles on the right side of the color bar, the handle (arrowhead) will appear with no fill color. When adjustment is complete right click on the handle to accept (resolve) the changes.

2. Assign red, green, and blue to the individual map regions, as follows:
  - a. Click on the map so the title above it (e.g., Si2) is green. The green title color indicates that it is selected.
  - b. Click on the arrow in the color option menu on the left side of the lower toolbar. The drop-down menu is displayed.
  - c. Click on the color to be assigned to the selected map region: red for the Si2 region, green for the Au3 region, and blue for the Ta2 region.
  - d. Repeat steps a, b, and c until the three colors have been assigned.
3. Adjust the image contrast and brightness for each map, as follows:
  - a. Click and drag the *upper* handle on the *right* side of the color bar down until the areas where the element is present are all or mostly white, and the areas where the element is absent show no or almost no white.

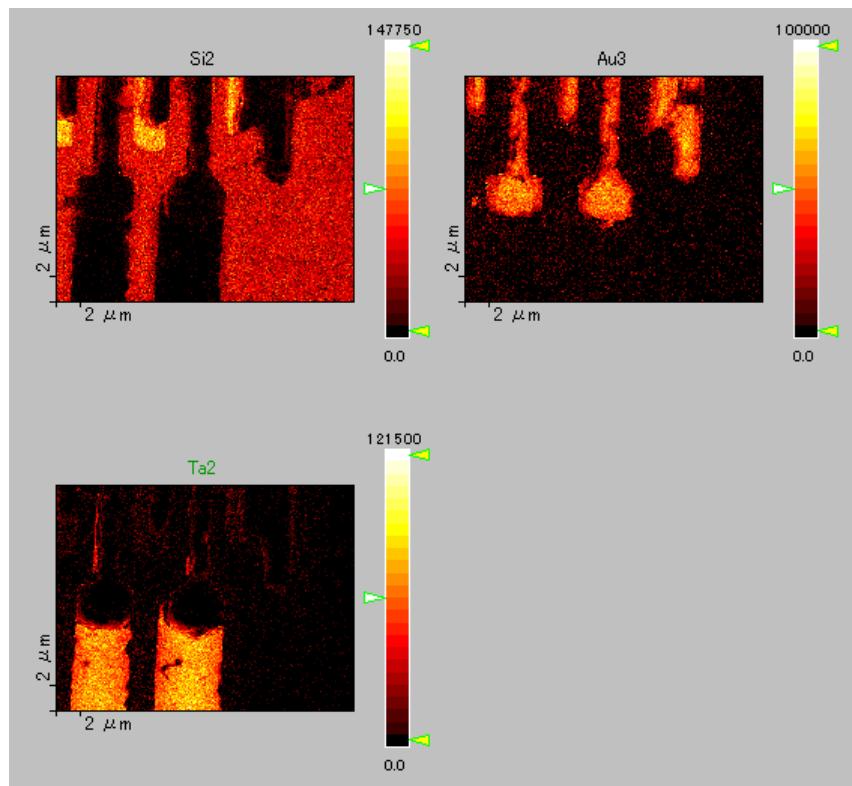
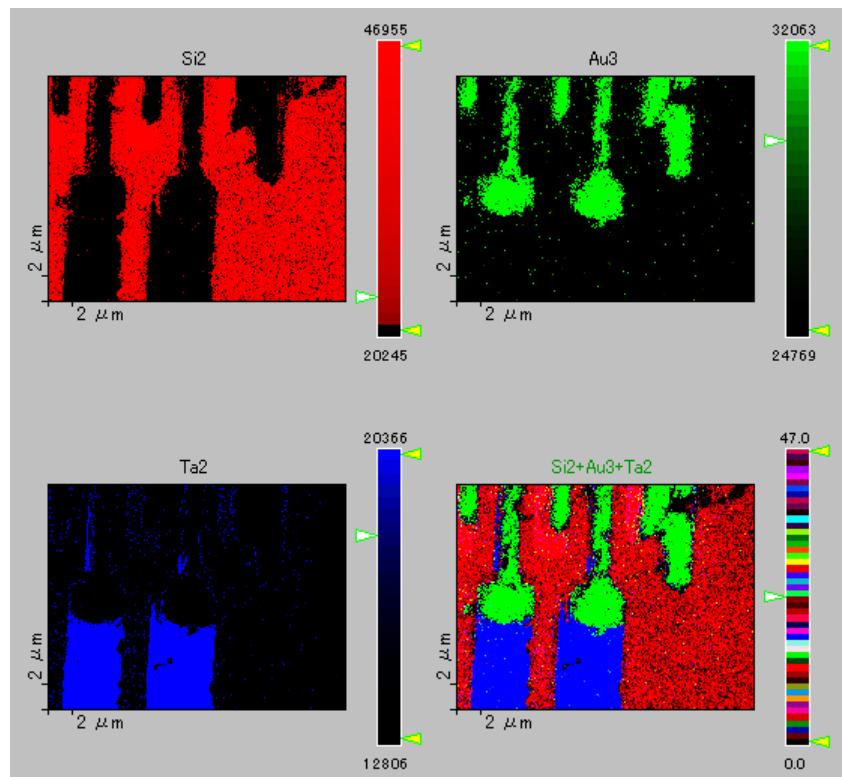


Figure 2-18. Map Window when "AUGERMAP.MAP" Is Opened.

- b. With the right mouse button click on the upper handle to accept (resolve) the change in image contrast. The areas that appeared white during the contrast adjustment will be displayed with a high intensity of the selected color after the contrast change has been accepted. The easiest way to undo this a contrast change is to Close and Reopen the map data file.
- c. Click and drag up the lower handle on the right side of the color bar until the areas where the element is not present are mostly black.
- d. With the right mouse button click on the lower handle on the right side of the color bar to accept (resolve) that operation.
- e. Click and drag the handle on the left side of the color bar for optimum brightness.
- f. Repeat steps a through e for each of the three maps.

The result should look very similar to the first three maps in Figure 2-19. Select File-Close and Reopen to reload the original maps if you wish to reprocess them.



*Figure 2-19. After Adjusting the Contrast and Brightness and Selecting Tools–RGB Overlay.*

4. To create a three color composite image of the three maps select Tools–RGB Overlay. The red-green-blue overlay of the three map regions, titled “Si2+Au3+Ta2,” will be displayed as shown in Figure 2-19.
5. Add text to the overlay image to identify the element associated with each color, as follows:
  - a. Select (click on) the RGB overlay image, if it is not already selected. (When it is selected, its title will be displayed in green.)
  - b. Turn off (unchecked) the Tile check box in the upper toolbar to display only the current image in the viewer.
  - e. Click on the image and type “Si = red <Enter> Au = green <Enter> Ta = blue.” The result is shown in Figure 2-20. If desired, text can be repositioned by clicking on it and dragging it to the desired location.

## 2: Getting Started

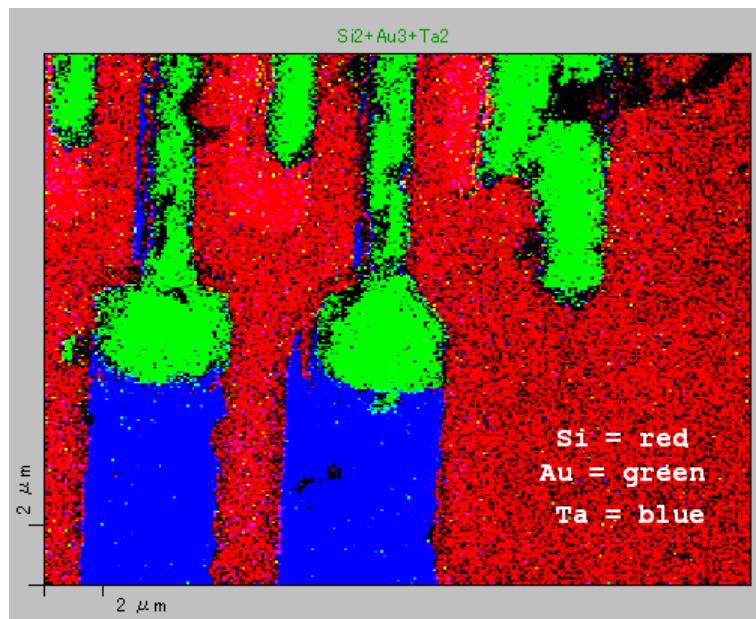


Figure 2-20. Color overlay image with annotation.

## PC Tutorial—Data Reduction of XPS Data Files

This section describes typical analyses of an XPS spectrum, an XPS depth profile, and an XPS map *using MultiPak*. The tutorial uses the files PET.SPE, XSPSPROF.PRO, and TONER.MAP, which are installed during installation of the MultiPak software.

### **Analyzing an XPS Spectrum**

In the following example, the file PET.SPE is used to demonstrate (1) refining the limits of analysis regions, (2) displaying MultiPak's "properties dialog boxes," and (3) curve fitting.

1. Open the ESCA spectrum file, as follows:

- a. Select File—Open. The Open dialog box is displayed.
  - b. Select .SPE or \*.\* in the File Type field, then double-click on PET.SPE (or click on the file name so it becomes highlighted, then click on OK). This file is a multiplex file with data from the carbon (C1s) and oxygen (O1s) regions.

The data is displayed in the Spectrum window. Notice that the file's name is displayed in green, indicating that this data is selected as the current file. Any MultiPak functions activated will be applied to this data.

The file header lists the file's data acquisition parameters (date of acquisition, x-ray beam conditions, analyzer pass energy, etc.). The two element regions, C1s and O1s, are listed in the region bar below the spectra display and their region buttons are currently turned off.

2. Click the C1s region button in the region bar of the Spectrum window, and adjust the region boundaries (vertical cursors), as follows:

- a. Click and drag the left region boundary to ~292 eV.

Notice that the Energy field in the lower toolbar indicates the location of the cursor along the x axis.

The dashed line displayed between the boundaries during the drag is the background curve. (See the next step.)

- b. Click and drag the right region boundary to ~280 eV.

The data should look like that shown in Figure 2-21.

## 2: Getting Started

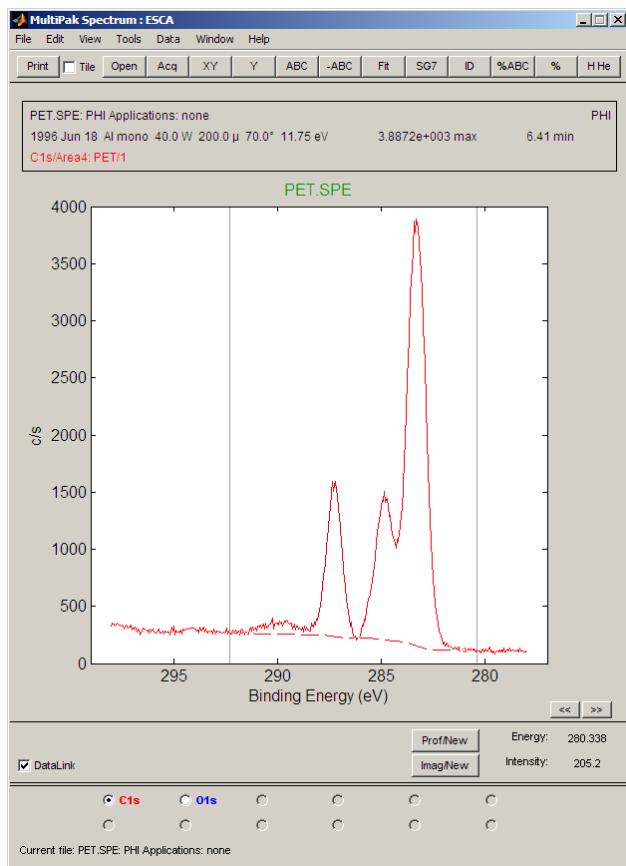


Figure 2-21. The C1s Region after Adjusting the Region Boundaries.

3. Use the mouse to practice displaying the MultiPak properties dialog boxes, as follows:
  - a. While depressing the Shift key, click on the right or left region boundary line with the left mouse button ([Shift]-left click). The Analysis Region Properties dialog box (Figure 2-22) is displayed. From this dialog box the spectral background type (Figure 2-23) and Peak Intensity measurement mode can be viewed or selected. Press OK or Cancel to close the dialog box.
  - b. [Shift]-left click on the data curve. The Data Properties dialog box (Figure 2-24) is displayed. From this dialog box the properties of the displayed data curve can be viewed or changed. Press OK or Cancel to close the dialog box.
  - c. [Shift]-left click on the x or y axis. The Axis Properties dialog box (Figure 2-25) is displayed. From this dialog box the scale of the axis and the axis labels can be viewed or changed. Press OK or Cancel to close the dialog box.
  - d. [Shift]-left click on the C in the Periodic Table window. The

## 2: Getting Started

Transition Properties dialog box for the C1s region (Figure 2-26) is displayed. (The terms “transition” and “region” are used interchangeably.) Press OK or Cancel to close the dialog box.

e. To view the properties for a specific C peak click on the arrow in the Transition pull-down menu near the top of the dialog box. Select “p->CKLL” from the list to view the Analysis Region Properties for the C KLL region as shown in Figure 2-27. Press OK or Cancel to close the dialog box.

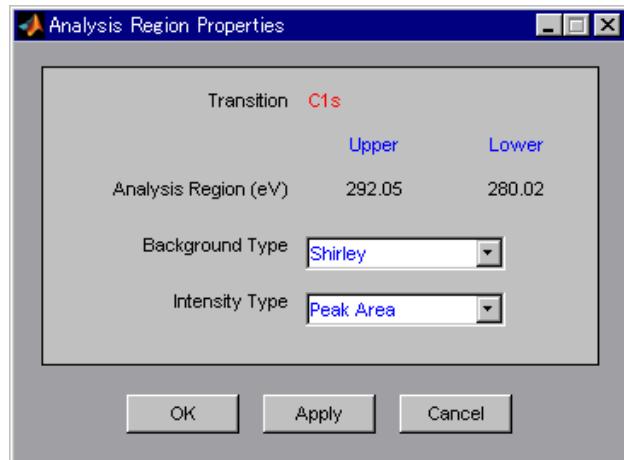


Figure 2-22. Analysis Region Properties Dialog Box.

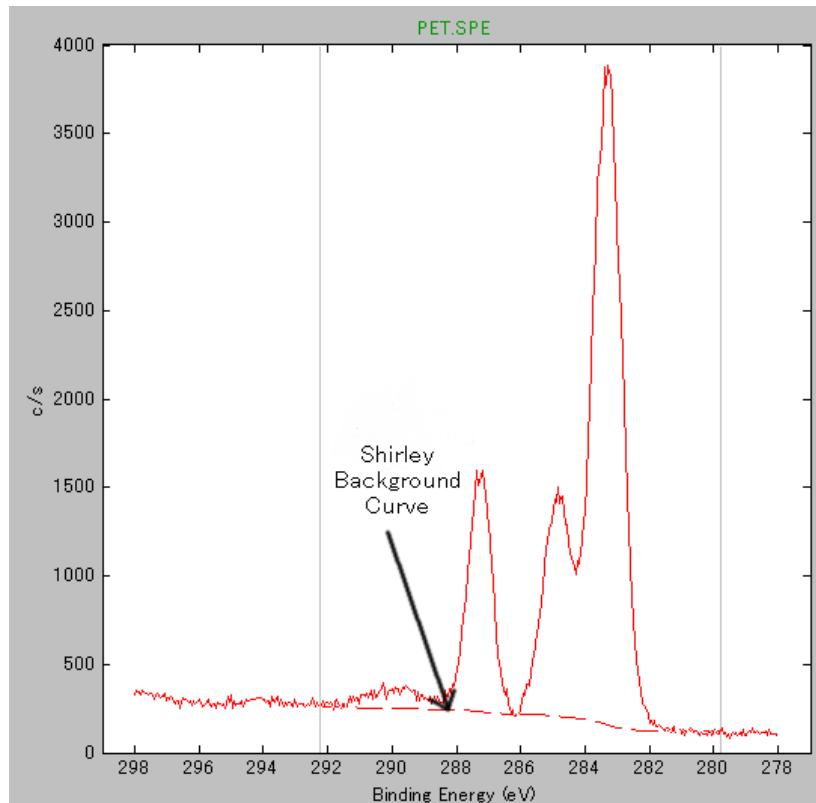


Figure 2-23. Illustration of a Background Curve.

## 2: Getting Started

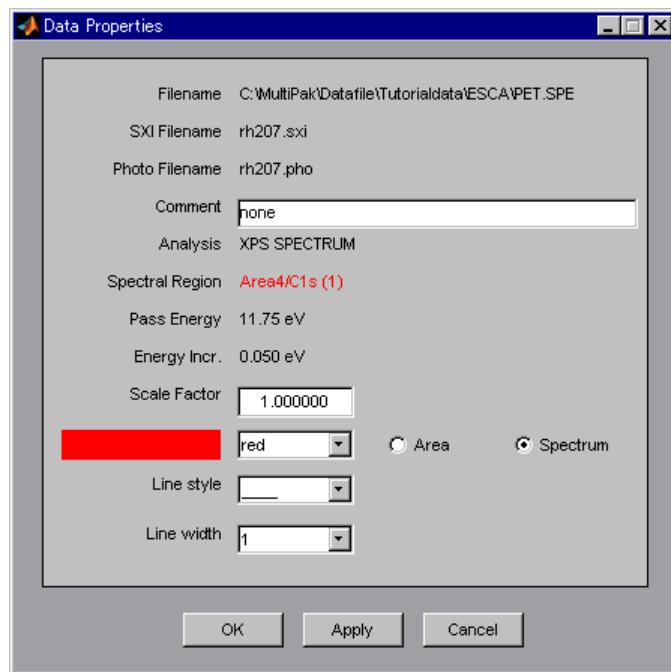


Figure 2-24. Data Properties Dialog Box.

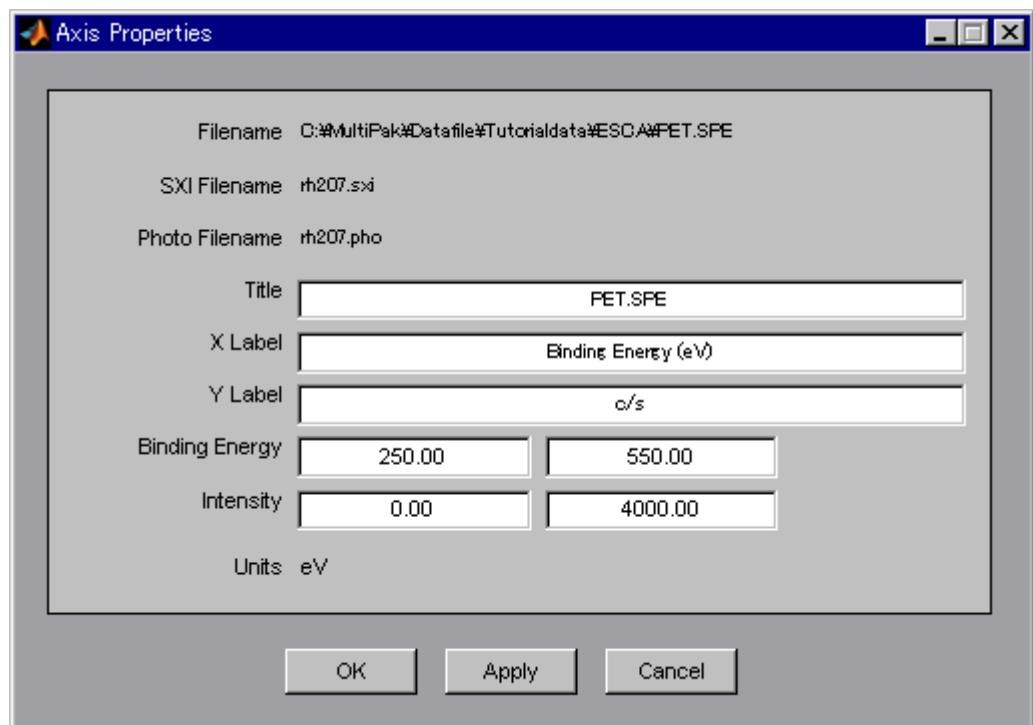


Figure 2-25. Axis Properties Dialogue Box.

## 2: Getting Started

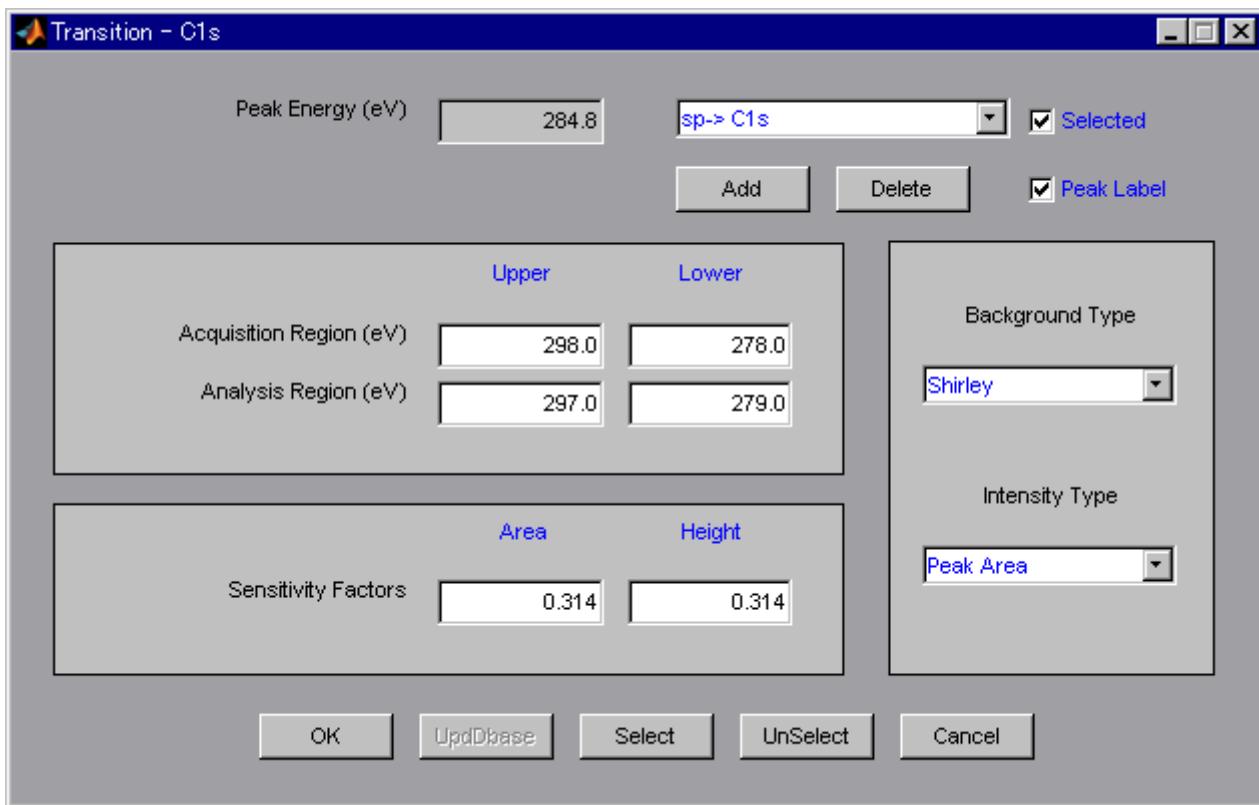


Figure 2-26. Transition (region) Properties Dialog Box for C1s.

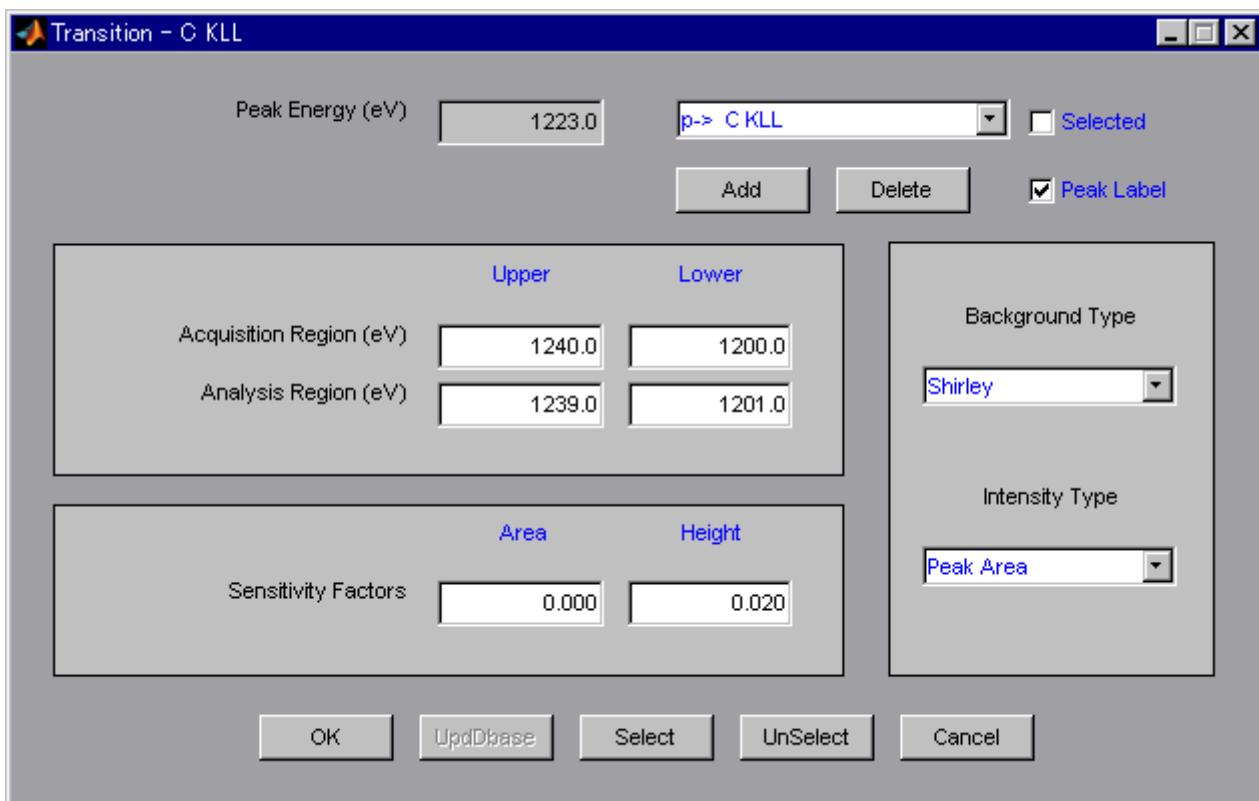


Figure 2-27. Transition Properties Dialog Box for C KLL.

## **2: Getting Started**

4. Perform a Curve Fit, as follows:
  - a. Press the Fit button in the upper toolbar. The lower toolbar and the Curve Fit Setup dialog box open.
  - b. Click on the Setup check box if it is not already set to on.
  - c. Select “Gauss-Lorenz,” peak shape if it is not already selected in the peak shape pull down menu at the top of the dialog box.
  - d. Click and drag the right mouse button to place a curve on each of the four peaks in the C 1s region.
  - e. If necessary each of the curve fit bands can be adjusted by first clicking on the band and then clicking and dragging the flags at the top and right hand side of the selected curve. It is also possible to manually enter values in the Curve Fit Setup dialog box. Figures 2-28 and 2-29 show the data and Curve Fit Setup menu after defining the curve fit bands.
  - f. Press the Fit button in the lower toolbar. Figure 2-30 shows the Curve Fit Setup dialog box and Figure 2-31 shows the data after the curve fitting process has been completed.
  - g. To display a summary of the curve fit press the View Sum button in the lower toolbar. Figure 2-32 shows the summary displayed in Notepad window.
5. When finished with the curve fit press the Exit button in the lower toolbar.

## 2: Getting Started

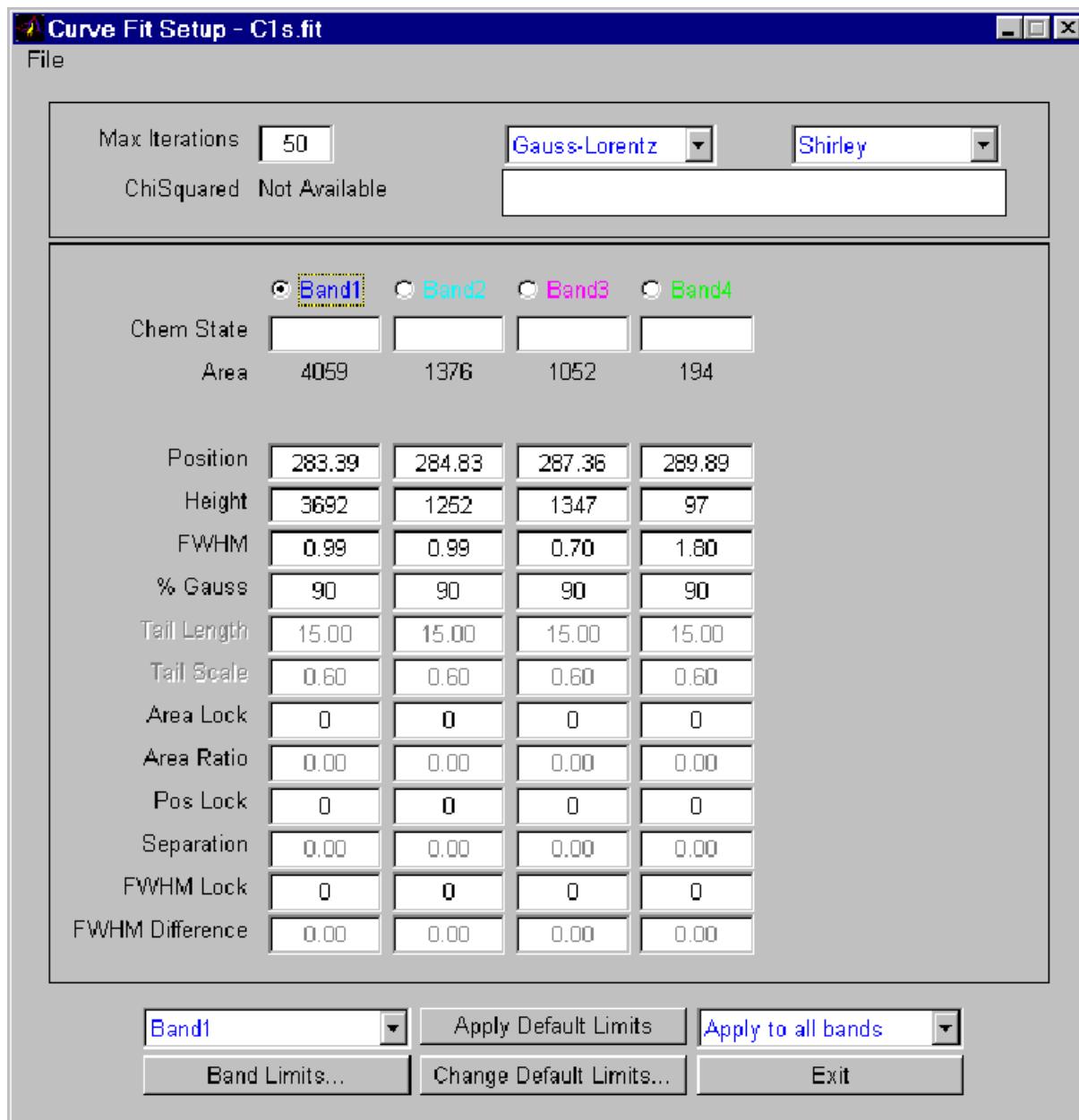


Figure 2-28. Values in the Curve Fit Setup Dialog Box before Pressing Fit in the Lower Toolbar.

## 2: Getting Started

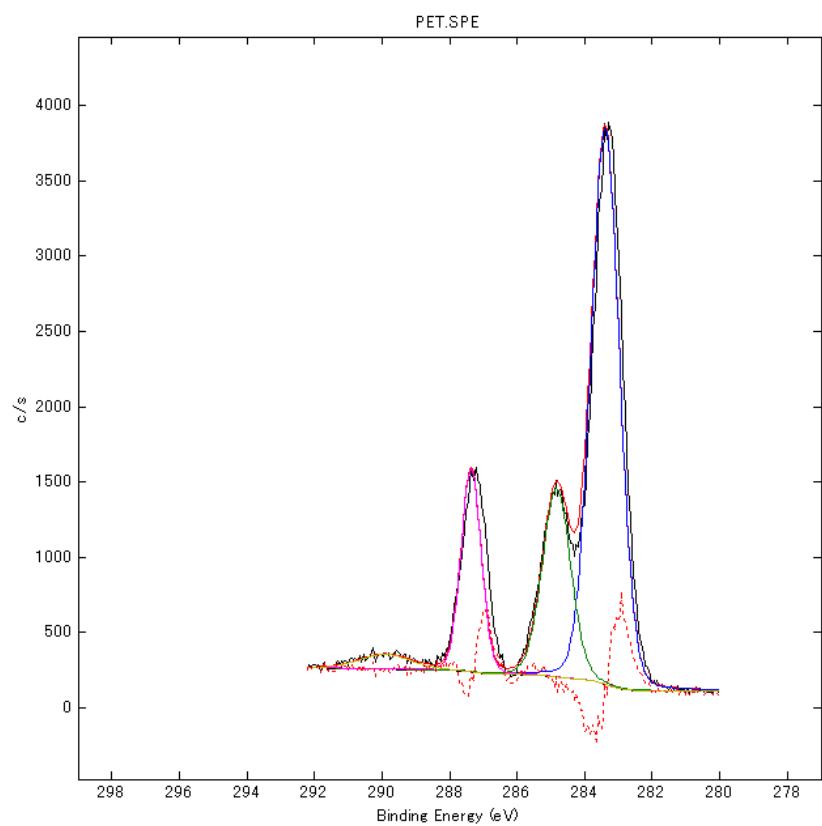


Figure 2-29. The four Curves (Bands) before Pressing Fit in the Lower Toolbar.

## 2: Getting Started

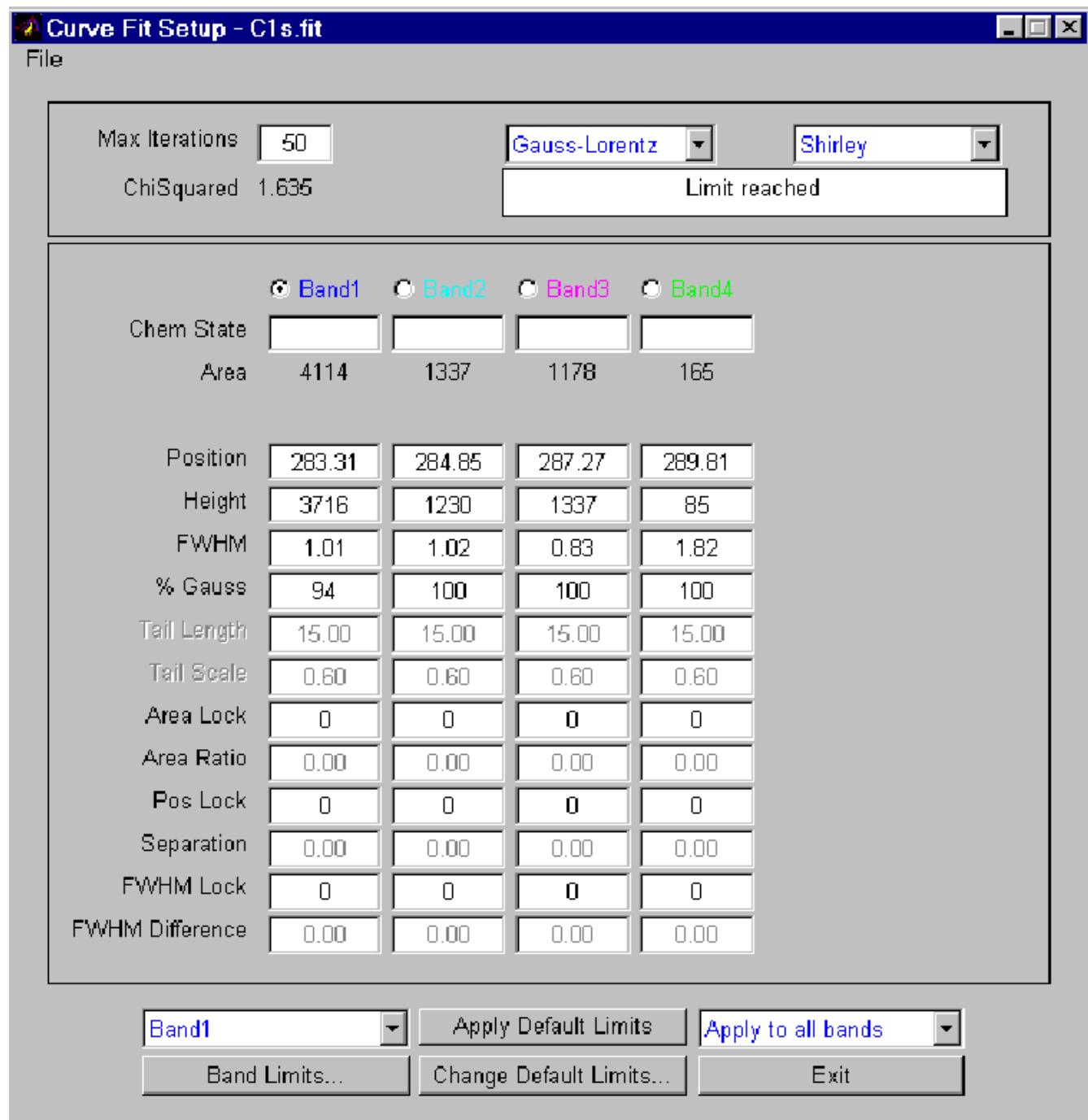


Figure 2-30. Values in the Curve Fit Setup Dialog Box after Pressing Fit in the Lower Toolbar.

## 2: Getting Started

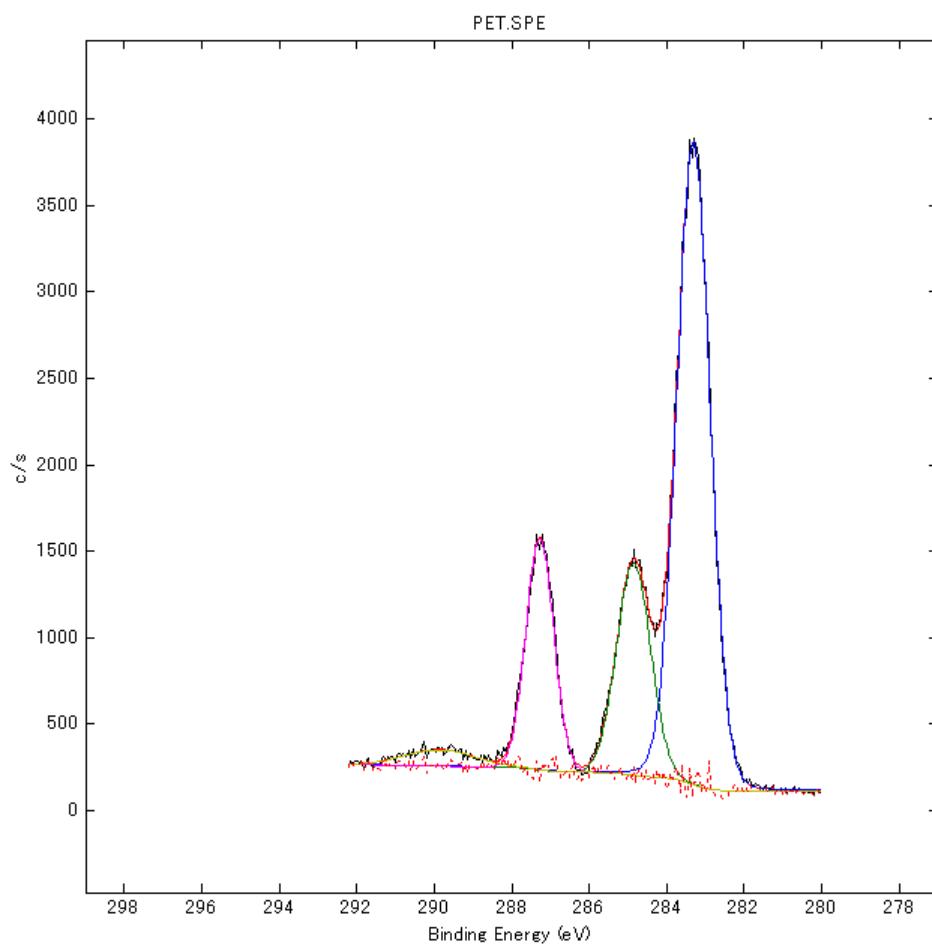


Figure 2-31. The four Curves (Bands) after Pressing Fit in the Lower Toolbar.

Spec Band	Pos	PosSep	B_FWHM	FWHM	Height	%Gauss	Area	%Area	ChiSquared
1	283.31	0.00	0.99	0.99	3728	90	4098	61.07	2.81
2	284.84	1.53	0.96	0.96	1229	90	1318	19.63	
3	287.28	3.97	0.78	0.78	1349	90	1173	17.48	
4	289.92	6.61	1.34	1.34	82	90	122	1.82	

Figure 2-32. The Curve Fit Summary Displayed in a Notepad window.

### Analyzing an XPS Sputter Depth Profile

In the following example, the file XPSPROF.PRO will be analyzed using the Linear Least Squares Fit function. The thin film sample consists of a W layer on top of a TiN and possibly a Ti layer on a Si wafer. In the depth profile window it appears that W is present in the TiN layer. We will use LLS to determine if W is actually present in the TiN layer. We will also use LLS to determine if a Ti layer is present at the interface between the TiN layer and the Si substrate.

1. Select File—Open. The Open dialog box is displayed. Select .PRO or \*.\* in the File Type field, then double-click on XPSPROF.PRO (or click on the file name so it becomes highlighted, then click on OK). The file will open in the Spectrum and Profile windows.
2. Click on the LLS button in the upper toolbar of the Profile window. The LLS toolbar (Figure 2-33) is displayed below the profile display.
3. Click on the W4f curve or click on the “W4f” in the upper right corner.
4. Define two subregions in the W4f energy range by clicking, dragging, and releasing the mouse twice. One region should be within the W layer and the other in the TiN layer where the W appears to be present. Figure 2-34 shows the appropriate boundaries of the two subregions. (Click on any region boundary with the right mouse button to adjust its position.) The spectra from these selected regions will be used as reference spectra to fit the raw data for W at each depth.
5. Press the Fit button in the lower toolbar. The result is shown in Figure 2-35. Note: in Version 9 of MultiPak the fitting will occur automatically it is not necessary to press the Fit button.

## 2: Getting Started

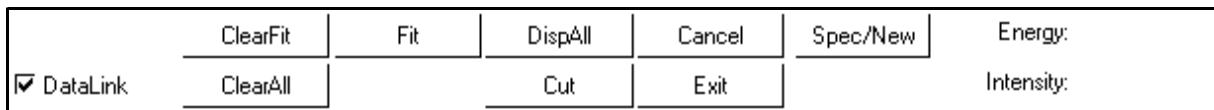


Figure 2-33. Linear Least Squares Fit Toolbar.

6. Turn on the Data Link check boxes in the lower toolbar of the Profile and Spectrum windows (if they are not on already), and turn off the Tile check box in the upper toolbar of the Spectrum window (if it is not off already).
7. Press the Spec/New button in the lower toolbar of the Profile window.

The Spectrum window displays a “View Only” rendering of the two reference spectra (Figure 2-36) created from the data in the two sub regions. The reference spectrum from the W layer is W 4f and the reference spectrum from the TiN layer is not W, it is a Ti 3p spectrum from the Ti in the TiN layer. This peak overlap between Ti and W can be removed using LLS fitting.

8. Press Exit in the lower toolbar of the Profile window to close the LLS function.

The profile now shows two additional regions, called W4f.ls1 and W4f.ls2, as shown in Figure 2-37. W4f.ls1 is the tungsten curve without titanium and W4f.ls2 is the titanium curve.

## 2: Getting Started

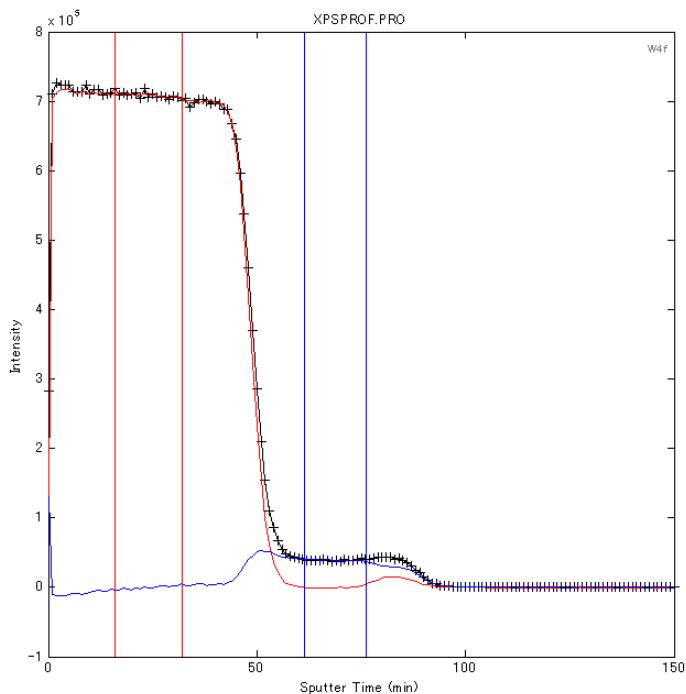


Figure 2-34. Two Subregions Defined in the W4f Profile.

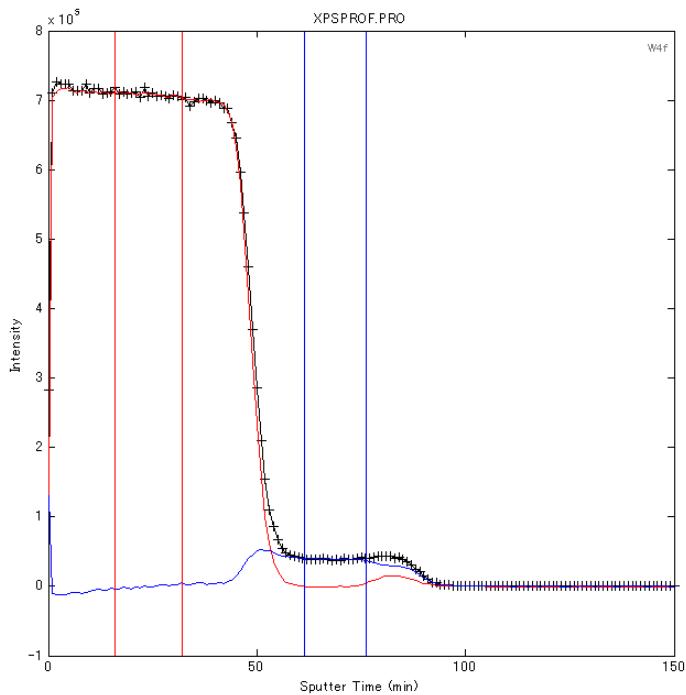


Figure 2-35. Result of LLS Fit on the Two Subregions.

## 2: Getting Started

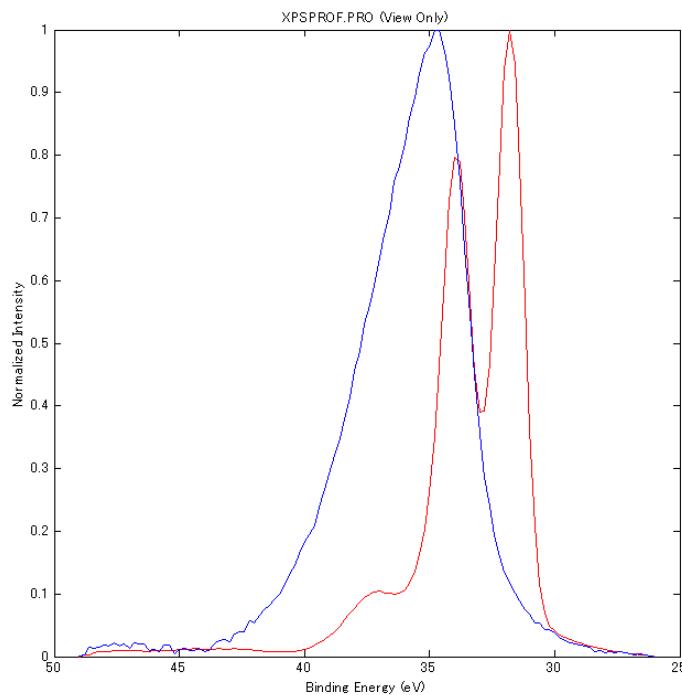


Figure 2-36. Spectra from the Two Subregions.

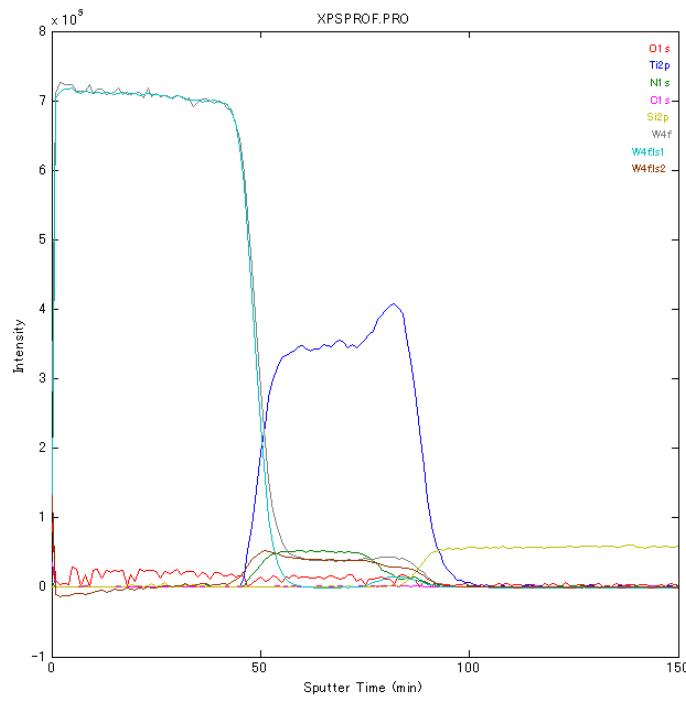


Figure 2-37. XPS PROF.PRO with Two New Profiles Generated by the LLS Function.

10. Press LLS on the upper toolbar again. Click on the Ti2p curve or on “Ti2p” in the upper right corner.

## **2: Getting Started**

The Ti2p energy range is displayed in the Profile window, with “+” marks showing every point along the curve. Because this is a depth profile, a spectrum is associated with each “+.” The two subregions from the previous LLS are also still displayed.

11. Press Cut, then press Cut again in the lower toolbar to remove the two sub regions remaining from the previous LLS fit. Figure 2-38 shows the Ti2p region after the cuts.
12. Define two very narrow subregions in the Ti2p energy range by clicking, dragging, and releasing the left mouse button. Figure 2-39 shows the appropriate boundaries of the two new subregions. (Click on any region boundary with the right mouse button to adjust its position.)

The Spectrum window is automatically refreshed with spectra for the two subregions, since in the lower toolbar of the Profile window the Data Link button is set to on and the Spec/Upd button is displayed instead of the Spec/New button.

In the Spectrum window (Figure 2-40), the two peak shapes are very similar but their peaks are shifted, indicating two chemical states of titanium are present in the region. Further examination reveals that the peak at the higher binding energy is TiN and the other is metallic Ti.

13. Press the Fit button in the lower toolbar. The result is shown in Figure 2-41. Note: in Version 9 of MultiPak the fitting will occur automatically it is not necessary to press the Fit button.
14. Press Exit in the lower toolbar of the Profile window to close the LLS function.

The profile now shows two more regions, labeled Ti2p.ls1 and Ti2p.ls2. Ti2p.ls1 is TiN, and Ti2p.ls2 is Ti (Figure 2-42).

15. In the lower toolbar of the Profile window, turn off the W4f.ls2, Ti2p, and W4f region check boxes, since these data are already better represented by the new curves W4f.ls1, Ti2p.ls1, and Ti2p.ls2.

## 2: Getting Started

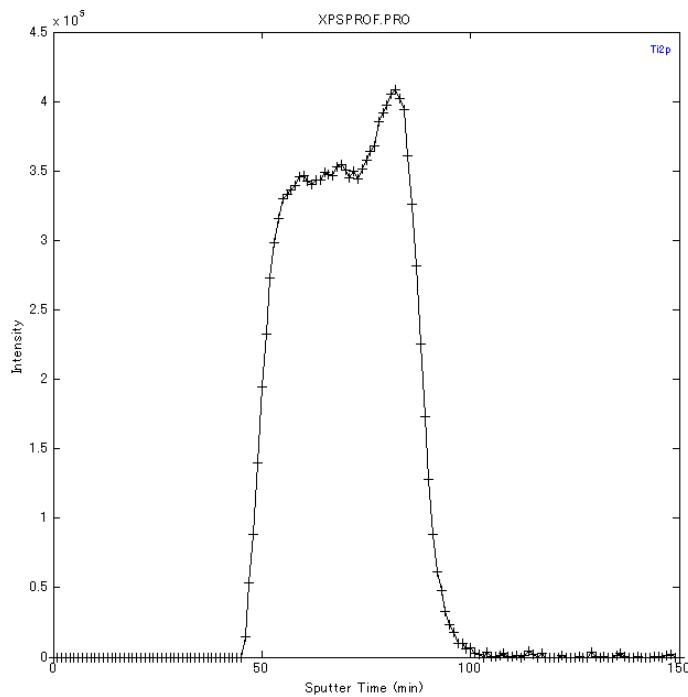


Figure 2-38. The Ti2p Profile in XPSPROF.PRO.

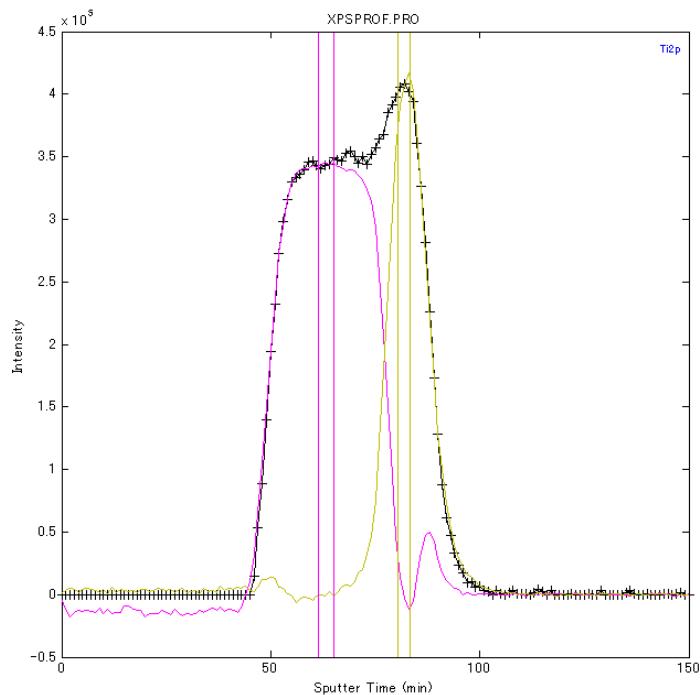


Figure 2-39. The Ti2p Profile with Two Subregions Defined.

## 2: Getting Started

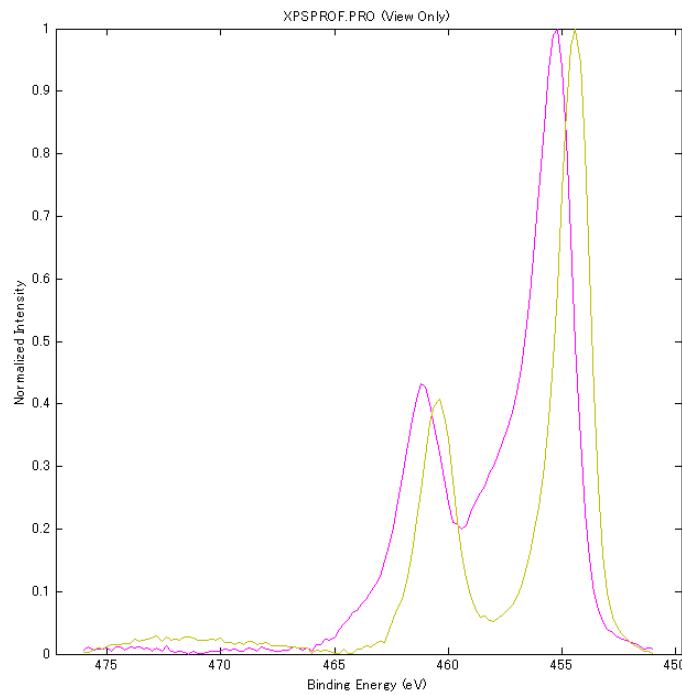


Figure 2-40. Spectrum Window Showing the Spectra from the Two Subregions.

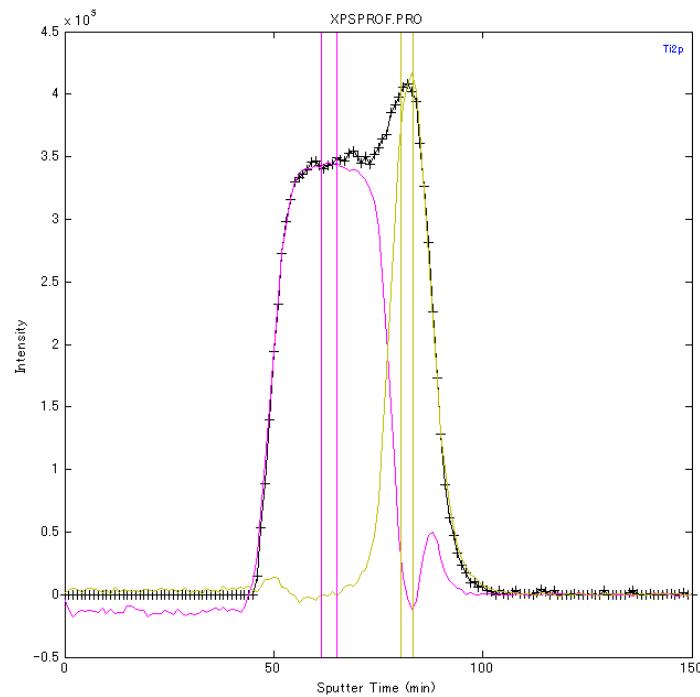


Figure 2-41. Result of LLS Fit on the Two Subregions.

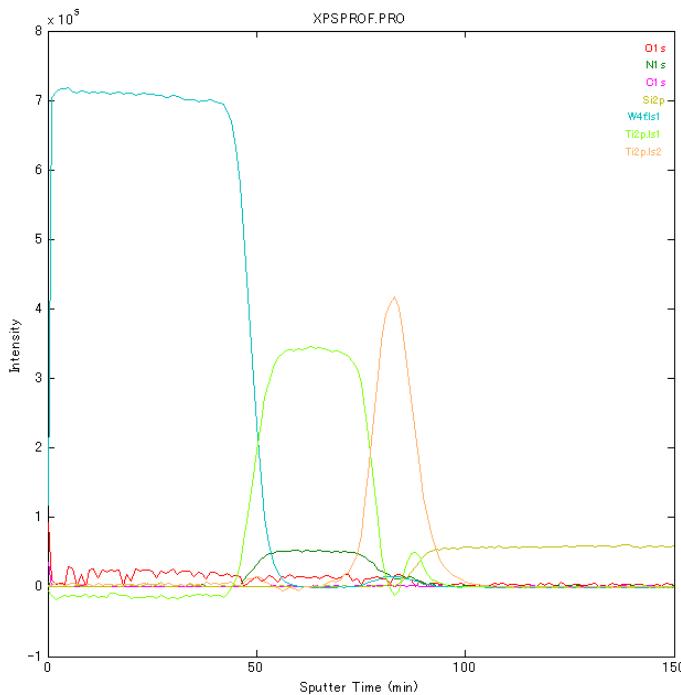


Figure 2-42. XPSPROF.PRO with the Three New “Regions” Created by LLS.

### Analyzing an XPS Map

In the following example, the file TONER.MAP is analyzed using the Linear Least Squares Fit routine and adjusting the contrast and brightness. The map is of a character printed on paper with toner.

1. Open the file TONER.MAP, as follows:
  - a. Select File—Open. The Open dialog box is displayed.
  - b. Select .MAP or \*.\* in the File Type field, then double-click on TONER.MAP (or click on the file name so it becomes highlighted, then click on OK). The file opens in the Map window.
2. In the lower toolbar of the Map window, click on the arrow in the colors option menu, then click on “pseudo,” and turn the Data Link check box on, if it is not already on.
3. In the lower toolbar of the Spectrum window, turn the Data Link check box on, if it is not already on, and select the C1s region (click on its button).
4. [Shift]-left click on one of the C1s region boundaries (vertical cursors in the Spectrum window). The Analysis Region Properties dialog box opens.

## 2: Getting Started

5. In the Analysis Region Properties dialog box, click on the arrow in the Intensity Type option menu, then click on “COG” (center of gravity). Press OK.

Figure 2-43 shows the Analysis Region Properties dialog box, Figure 2-44 shows the Spectrum window display, and Figure 2-45 shows the Map window display.

6. In the Spectrum window, drag the left boundary of C1s to ~292, and drag the right boundary to ~277.
7. Press LLS in the upper toolbar of the Map window.
8. Select Rectangle in the LLS toolbar, if it is not already selected.
9. Click and drag on the map to create two subregions, as shown in Figure 2-46.

Use the Cut button to remove any region that was drawn incorrectly.

10. Press Fit in the LLS toolbar. Figure 2-47 shows the two images (maps of each subregion) that are added to the display.
11. Press Exit in the LLS toolbar.

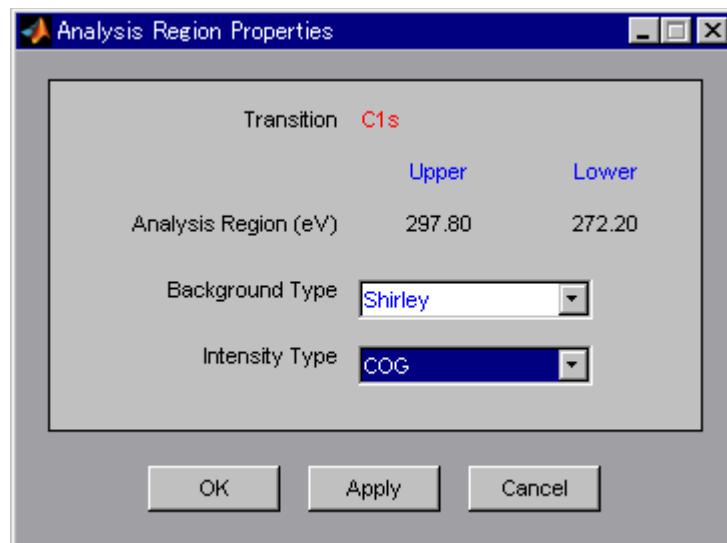


Figure 2-43. Analysis Region Properties Dialog Box for C1s.

## 2: Getting Started

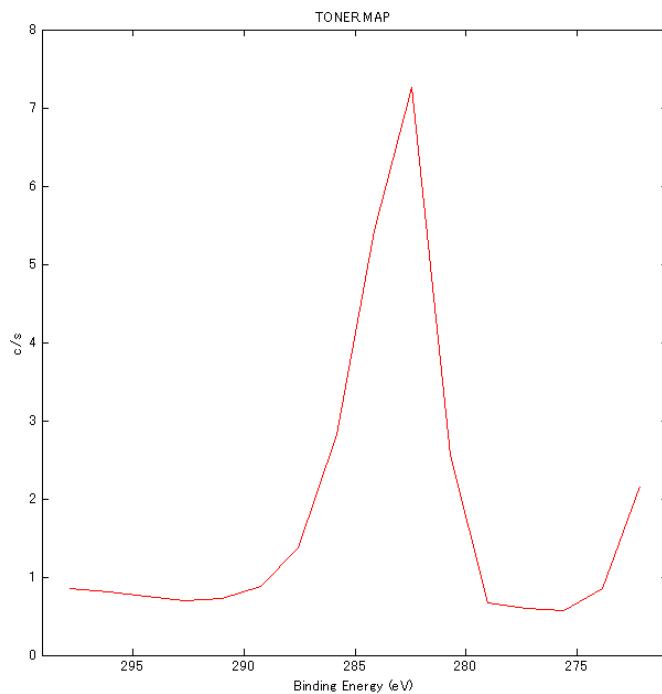


Figure 2-44. Spectrum Window Display of TONER.MAP.

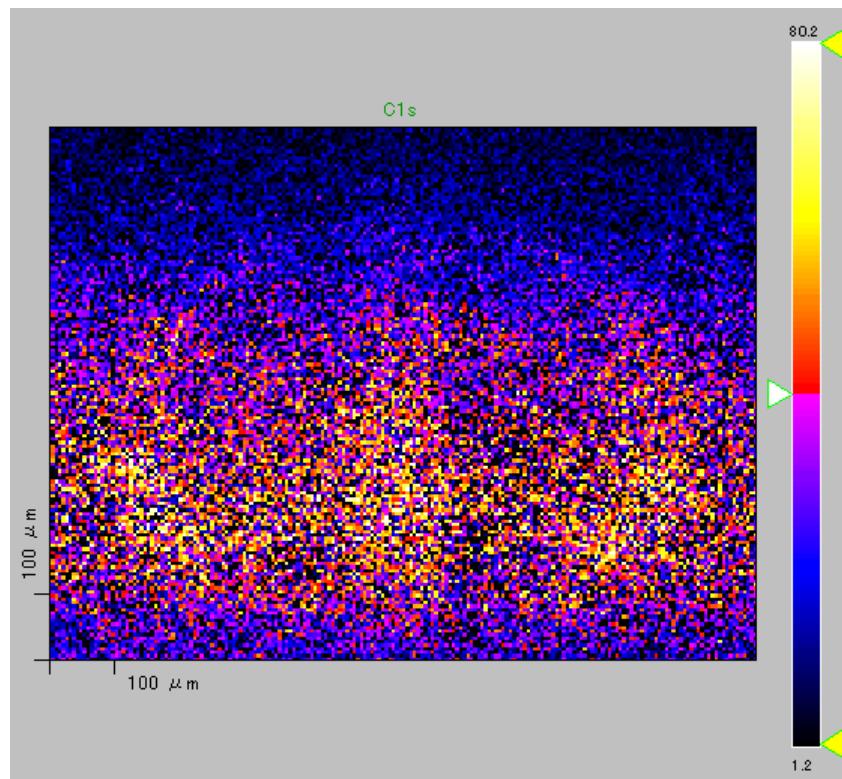


Figure 2-45. Map Window Display of TONER.MAP.

## 2: Getting Started

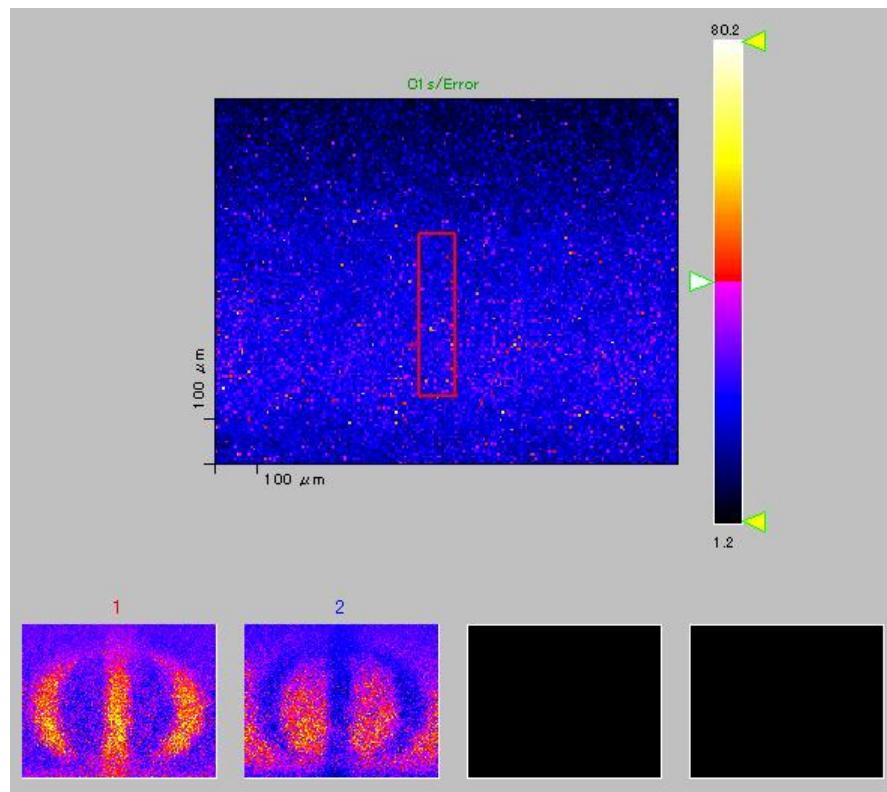


Figure 2-46. Two Subregions Drawn on TONER.MAP. Note: the blue subregion on the right is difficult to see.

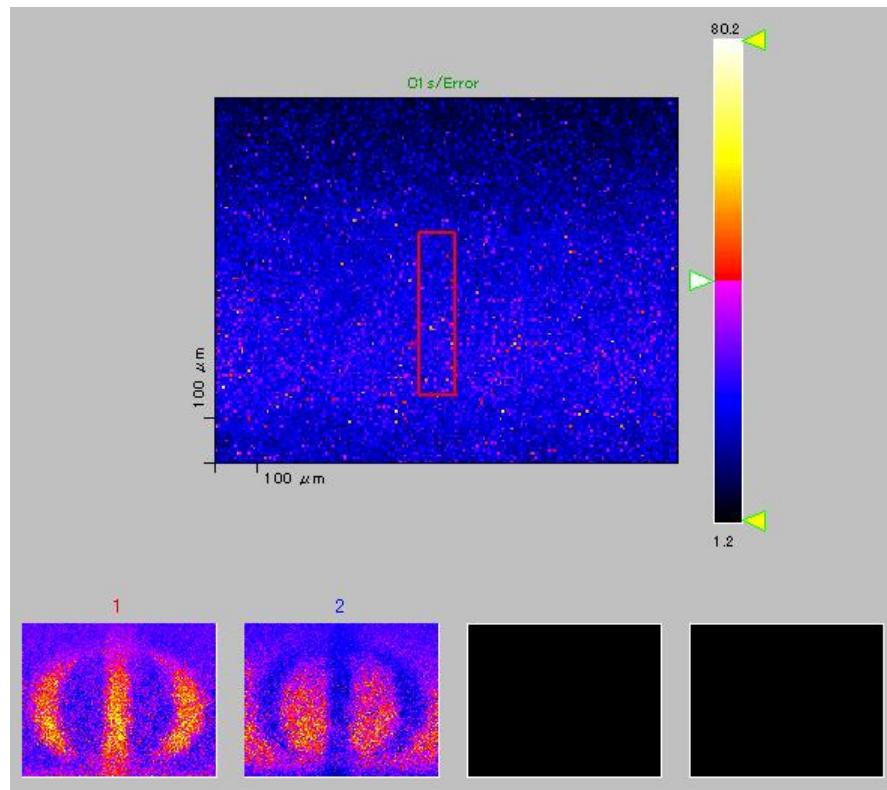


Figure 2-47. Maps of the Two Subregions after Fitting with LLS.

## 2: Getting Started

12. Click on the map titled “C1s.ls1.” (C1s.ls2 could be used instead.)
13. Turn off the “Tile” check box in the upper toolbar of the Map window. The map of the subregion is displayed alone and larger in the Map window.
14. On the color bar to the right of the subregion map:
  - a. Drag the *brightness* arrow on the left, then release the mouse button. Repeat this until the best image (most contrast) is displayed.
  - b. Drag the top *contrast* arrow (on the right side of the color bar) down about half way. Then, click on it with the right mouse button to “resolve” (accept) the operation.
  - c. Drag the bottom *contrast* arrow (on the right side of the color bar) up about half way. Then, click on it with the right mouse button to “resolve” the operation. The result is shown in Figure 2-48.
15. Select other choices in the color option menu in the lower toolbar to see the results.

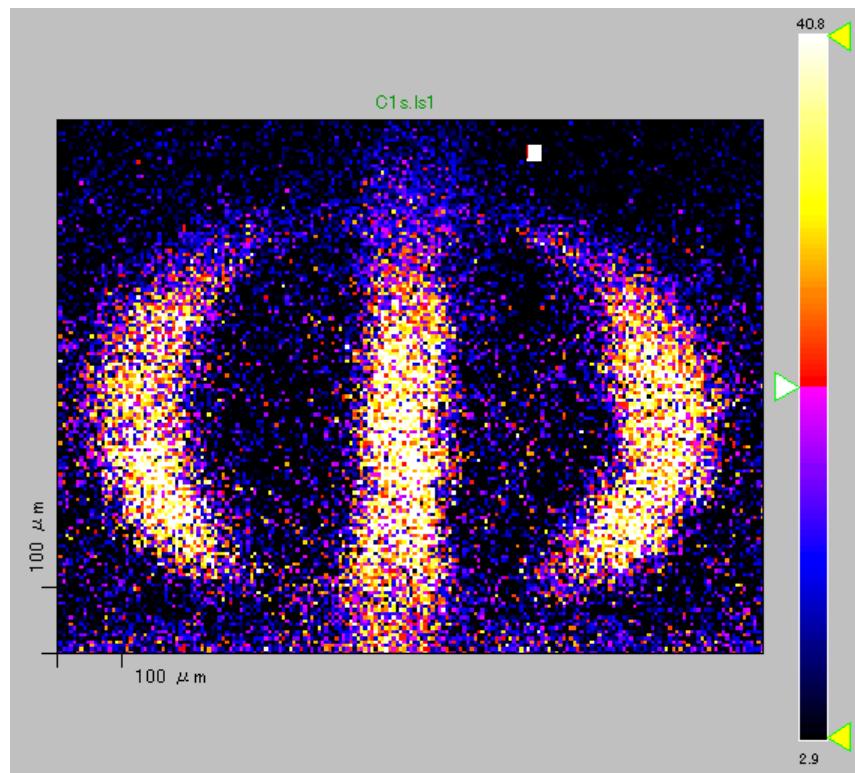


Figure 2-48. After LLS fitting and contrast adjustment the image of the toner is clearly visible on the paper is clearly visible.



## **Section 3: MultiPak Functions**

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Many MultiPak functions can be activated from more than one location. They could be listed on a menu, as a toolbar button, or as a selection in a dialog box. For this reason, Section 3 presents these functions according to name rather than according to how they are accessed. Generally, the names of pushbuttons in the upper and lower toolbar and in dialog boxes are in bold letters.

### **%**

The percent (**%**) pushbutton, available in the upper toolbar of the Spectrum and Profile windows, generates an atomic concentration table according to the selections in the Atomic Concentration Table Format dialog box.

*See also AC%; Atomic Concentration Table.*

### **%ABC**

The **%ABC** pushbutton, available in the upper toolbar of the Spectrum window, generates a simple atomic concentration table for the currently selected spectrum and places it in the upper right corner of the axes as annotation.

*See AC%; Annotate...; Atomic Concentration Table.*

### **Å**

*See X-Axis Scale.*

### **ABC, -ABC**

These buttons, available in the upper toolbar, start the Annotate... function (**ABC**) and remove all annotation (**-ABC**) from the current axes.

*See also Annotate...; Clear All Annotation; Clear Annotation.*

## About MultiPak

The About MultiPak function, which is on the Help menu, displays the version of the MultiPak software and the copyright information.

### AC%

When the AC% check box in the Profile and Map upper toolbars is on (checked), the data are displayed in percent atomic concentration (Figure 3-1). When the check box is off, the data are displayed in intensity (units), as shown in Figure 3-2.

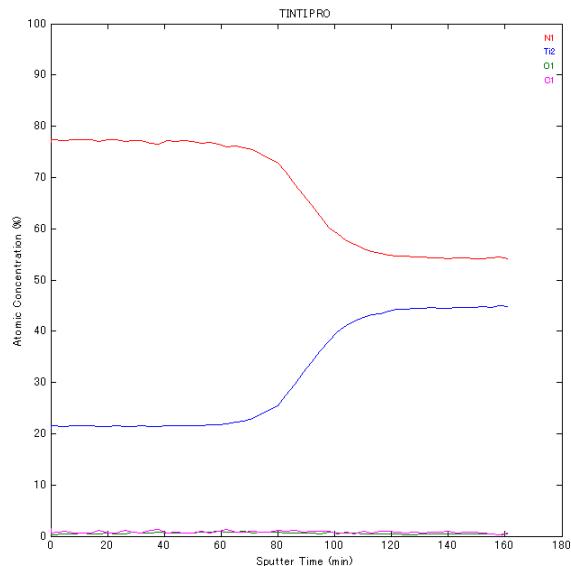


Figure 3-1. Data Axes When AC% Is On.

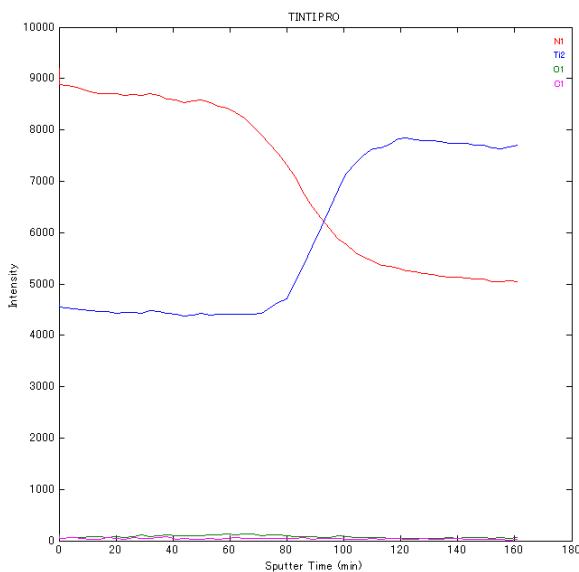


Figure 3-2. Data Axes When AC% Is Off.

## Acq

Pressing the **Acq** button on the upper toolbar (or selecting File–Open Last Acquisition) automatically finds and opens the data acquisition file most recently created by instrument control software. When regions are defined for the acquisition, those region buttons are displayed in the region toolbar and those elements are turned on automatically in the Periodic Table.

## Add/Subtract/Compare...

Selecting Add/Subtract/Compare... from the Data menu of the Spectrum window displays a lower toolbar that allows the user to modify a spectrum by adding or subtracting another spectrum.

*NOTE: The display cannot be in Tile mode when the function is started.*

A “Reference” spectrum and “Source” spectrum are selected, the reference spectrum can be adjusted if desired, and the Reference spectrum is added to or subtracted from the Source spectrum.

To choose the Source spectrum, scroll through individual spectra using the selection slider. When the spectrum to be used as the Source is displayed, release the mouse button. The Source spectrum is displayed in red (when the Source check box is checked).

Once the Source spectrum has been defined, choose a Reference spectrum in one of the following ways:

- Use the selection slider to display individual spectra until an appropriate spectrum is found, then press the **SetRef** pushbutton in the lower toolbar.
- Press the **LoadRef** pushbutton in the lower toolbar, and double-click on another .SPE file. The first spectrum in that file becomes the Reference spectrum.

The Reference spectrum is displayed in green (when the Ref check box is checked) and the Add and Subtract buttons are enabled. The name of the .SPE file that the Reference spectrum came from is displayed in the lower left corner. Green range cursors, described below, are also displayed.

When the Source and Reference spectra have been chosen, the **Add** or **Subtract** button can be pressed or a different Source or Reference spectrum can be selected.

### 3: MultiPak Functions

*NOTE: The Reference and Result spectra are affected by operations even when they are not displayed.*

The green range cursors initially enclose the maximum overlap of the Reference spectrum with the Source spectrum. They can be dragged to different positions to indicate the range of the Reference spectrum that is to be used in the operation. Only the overlapped portions of the spectra are used in the Add/Subtract operation. The length of the Result spectrum, however, is the same as that of the Source spectrum.

*NOTE: When no portion of the Reference spectrum is between the range cursors, the range cursor is returned to its position prior to the move. When one cursor is beyond the end of the Reference spectrum, the energy of the Reference spectrum's end point is used. When both cursors are beyond the ends of the Reference spectrum, the entire Reference energy range is used.*

When the Reference spectrum is displayed and selected, it can also be modified according to the selection in the toolbar's option menu. The Energy and Intensity fields in the lower toolbar display the changes to the Reference spectrum as the mouse is dragged. Changing the Reference spectrum is done in one of the following ways:

- *Y-Offset* is used to apply a vertical correction to the Reference spectrum. Button down (clicking) establishes the reference point, and button up (releasing the mouse button after a *vertical* drag) establishes the difference in the Y direction from this reference point. This difference is used in the offset correction.
- *X-Shift* is used to shift the energy position of the Reference spectrum. (The green range cursors track with the movement of the Reference spectrum.) Button down (clicking) establishes the reference point, and button up (releasing the mouse button after a *horizontal* drag) establishes the difference in the X direction from this reference point. This difference is used to shift the Reference spectrum.
- *Y-Linear* is used to apply a linear correction to the Reference spectrum. The right range cursor identifies the anchor point on the Reference spectrum. Button down (clicking) on the 'left side' of the reference spectrum establishes the reference point, and button up (releasing the mouse button after a *vertical* drag) establishes the difference in the Y direction from this reference point. This difference is used in the linear correction.
- *Y-Scale* is used to scale the intensity of the Reference spectrum. Button down (clicking) establishes the reference point, and button up (releasing the mouse button after a *vertical* drag) establishes the difference in the Y direction from this reference point. This difference is used to scale the intensity of the reference spectrum.

### **3: MultiPak Functions**

Clicking and dragging the right mouse button causes:

- *ESCA*—Y-Offset and Y-Shift to happen at the same time.
- *AES*—X-Shift and Y-Scale to happen at the same time.

The **Source**, **Ref**, and **Result** buttons toggle the display of the associated spectrum between show and hide. Clicking the **OriginalSrc** button restores the current Source spectrum to its original values. Clicking the **OriginalRef** button undoes all adjustments to the Reference spectrum and returns the Reference spectrum to its original state (even if it is not displayed).

The Result spectrum can be saved in a file using the File—Save Current Spectrum As... function.

Clicking the **Cancel** button restores all Source spectra to their original values and exits the application. Clicking the **Exit** button exits the application but still displays the changes in Source spectra and, if the Data Link check box is on (checked), updates the displays of any associated profiles or maps.

*See also* Selection Slider....

## **Adjust Region Endpoints**

The Adjust Region Endpoints function may be selected from the Spectrum window's Tools menu, Spectrum Autoreduction Setup dialog box, or Select Spectra toolbar.

The function automatically repositions the endpoint cursors for the selected analysis region(s) based on data from the selected spectrum or from a composite spectrum that is generated from all selected spectra.

The process is performed on each region.

## AES

MultiPak is always in either ESCA or AES mode, indicating which type of data is currently being reduced. The File–Options menu of each main window allows switching between these two modes. Note: in Version 9 MultiPak will automatically switch modes when AES or ESCA files are opened.

All open files are automatically closed when the mode is switched.

ESCA stands for Electron Spectroscopy for Chemical Analysis, and is also known as X-ray Photoelectron Spectroscopy (XPS). AES stands for Auger Electron Spectroscopy, sometimes called Scanning Auger Microscopy (SAM).

## All

The All pushbutton in the region bar of the Profile and Map windows turns on all the region buttons.

## All Elements

*See* Energy Cursor.

## All Transitions

*See* Labels Option Menu.

## Analysis Region

Refer to “Periodic Table” for a description of the Analysis Region functions on the View menu.

*See also* Analysis Region Properties; Region; Region Cursors; Subregion; Transition Dialog Box.

## Analysis Region Cursors

*See* Region Cursors.

## Analysis Region Properties

Using [Shift]-left mouse button to select one of the region boundaries displays the Analysis Region Properties dialog box, which is used to view or change some information about the current region of the data, as follows:

- *Transition* displays the name of the current region (from the acquisition file);
- *Analysis Region (eV)* displays x-axis locations of the upper and lower boundaries of the region;
- *Background Type* displays the background calculation method;
- *Intensity Type* displays how the intensity is calculated.

The **OK**, **Apply**, and **Cancel** buttons work in the standard dialog box way.

*NOTE: Changes in these parameters affect the data within the currently selected analysis region.*

*NOTE: Changes made to the spectrum after the dialog box is opened are not reflected in the dialog box until it is closed and opened again.*

*See also* Appendix A, “Background”; Intensity Type; Region; Subregion; Transition Dialog Box.

## Annotate...

Selecting Annotate... from the Tools menu or upper toolbar (**ABC** button) displays a lower toolbar that allows the user to add text and lines anywhere within the selected data display or modify the style of different types of annotation. (See Clear Annotation to delete annotation.)

*NOTE: The user may also add text by clicking on a blank area within the axes and typing, without starting the Annotate function. This “free-form” annotation capability is also available during most other MultiPak functions.*

The “types” of annotation are listed in the toolbar’s right-most option menu. Each type has predefined default characteristics (styles). Using these styles helps standardize the look of printed results.

The option menus of the lower toolbar show the orientation (in degrees), font, size, style (normal, italic, etc.), and color for the type of annotation selected in the option menu. Any or all of the style attributes for a specific type of annotation can be changed using the option menus in the lower toolbar.

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The current settings are applied to *all* annotation on the selected data when the **Apply All** button in the lower toolbar is pressed, but only to the *selected* annotation when **Apply** is pressed.

The Ungroup button on the lower toolbar is used to separate text and its associated “marker” (line). This allows the markers (lines) and text to be moved independently from each other.

Pressing the **Exit** button closes the Annotate... toolbar.

Mouse functions during the Annotate... function are summarized in Table 3-1.

*NOTE: Up to 1,000 characters may be pasted from the clipboard by pressing [Ctrl][v] after clicking in the location where the text should be added to a data axes.*

*See also* Clear All Annotation; Clear Annotation; Energy Cursor; Labels Option Menu; Periodic Table; Text Properties.

Table 3-1. Mouse Functions during the Annotate... Function.

To:	Point At:	Press
Add annotation	where the text should begin	Left and type
Create line (“marker”) and associated annotation	where the line should begin	Left and drag to where the line should end, then type
Create second line of annotation	N/A	Press Enter after typing the first line, then continue typing
Select annotation	annotation within the axes	Left
Move annotation	annotation within the axes	Left & drag
Delete annotation	annotation within the axes	Left & drag outside the axes
Duplicate last typed or last highlighted annotation	text to be displayed	Right & drag to desired location
Change style (size, etc.) of annotation	annotation within the axes	[Shift]-Left

## Annotate Atomic Concentration

Selecting Annotate Atomic Concentration from the upper toolbar (%ABC button) or Tools menu calculates an atomic concentration table for the current spectrum and places it in the upper right corner of the data displayed.

See also Annotate...; Atomic Concentration Table.

## Area

This button is available on the upper toolbar of the ESCA Map window.

See Spatial Area.

## Area Comment

See Legend.

## Area Number

See Legend.

## Arial

See Annotate...; Text Properties.

## ASCII...

See Export To.

## Atomic Concentration

Atomic Concentration is available from the Data menu of the Profile and Map windows or the AC% check box in the upper toolbars. This function toggles the Y axis data display between peak intensity and percent concentration. (The Tools—Atomic Concentration Table functions generate atomic concentration data in the form of a *table*.)

When Atomic Concentration is selected, atomic concentration is calculated for all regions in the current axes (Profile window) or all maps current displayed (Map window) and (1) any negative values are changed to zeros, (2) intensities are calculated on the current data, and (3) results are displayed in the form of:

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- *Profile window*—Plot of time/distance/angle (x axis) vs. concentration (y axis).

*NOTE: The AES sensitivity factors used in the atomic concentration calculations on AES data are based on a 5-point differentiation. AES profile and line data must have a 5-point differentiation applied before performing AC calculations. (No other data reduction should be performed on the data before doing the AC.)*

*NOTE: AC calculations for AES data measured with the 4700TFA or Versaprobe II are performed with corrected sensitivity factors for SCA analyzers. See Appendix A for the correction calculation. Use 0.6% energy resolution data for AC calculations.*

- *Map window*—Set of maps of concentration at each x-y coordinate.

All atomic concentration maps will initially be displayed from 0% to the maximum concentration in that map. The scale can be changed using the map's contrast or threshold capabilities in a variety of ways, as described in Color Bar. (*See also Axis Properties.*)

*NOTE: Maps used to calculate atomic concentration can originate from different files, but the resolution of each map (e.g., 128 x 128) must be the same.*

*NOTE: Performing any operation on the data that changes the data set (e.g., changing the region end points) also changes the atomic concentration data. Also note that the region cursors should be adjusted to capture the correct peak area or peak height information prior to calculating atomic concentration.*

*See also Atomic Concentration Table; Appendix A, “Atomic Concentration.”*

## **Atomic Concentration Table**

Selecting Atomic Concentration Table from the Tools menu of the Spectrum or Profile window displays a cascading submenu: Clear, Add, View, Print, Recalculate, Quick Key Definition..., and Format....

Selecting *Clear* removes all AC results from the AC file. *Add* generates AC results and adds it to the AC file. *View* displays the data in the AC file using the default text file editor (Notepad). *Print* sends the data in the AC file to the printer. *Recalculate* generates new AC data and replaces the current AC data.

When MultiPak opens the text editor application to display the AC data, the contents of that file may be edited, added to, copied, printed, etc. (Refer to the documentation that came with your computer for information about

### 3: MultiPak Functions

using the text editor application.) Figure 3-3 shows an atomic concentration table for the file TINTI.PRO.

The diagram illustrates the structure of the TINTI.PRO file. It is divided into two main sections: the Header and the Atomic Concentration Table. The Header contains file information such as File Name: TINTI.PRO, File Type: AES DEPTHPRO, and Comment: TiN/Ti. The Atomic Concentration Table follows, with columns labeled Abscissa, C1, N1, O1, and Ti2. The table consists of 24 rows of data, each containing five values. A vertical bracket on the right side of the table is labeled 'Table', and a horizontal bracket at the top of the header section is labeled 'Header'.

Abscissa	C1 (0.076)	N1 (0.161)	O1 (0.212)	Ti2 (0.296)
0.00	19.48	65.53	1.49	13.50
0.00	19.66	65.37	1.53	13.44
5.00	19.75	65.30	1.50	13.46
8.00	19.60	65.42	1.51	13.47
11.00	19.72	65.28	1.52	13.48
14.00	20.10	65.04	1.51	13.36
17.00	19.69	65.29	1.53	13.49
20.00	19.87	65.28	1.46	13.39
23.00	20.11	65.01	1.57	13.31
26.00	19.77	65.36	1.48	13.40
29.00	19.84	65.18	1.55	13.43
32.00	19.76	65.12	1.64	13.48
35.00	19.73	65.36	1.47	13.45
38.00	19.73	65.28	1.47	13.52
41.00	19.75	65.32	1.43	13.50
44.00	19.78	65.34	1.41	13.47
47.00	19.75	65.18	1.58	13.49
50.00	19.81	65.30	1.44	13.45
53.00	19.66	65.34	1.42	13.57
56.00	20.11	64.82	1.51	13.55

Figure 3-3. Atomic Concentration Table for the File TINTI.PRO.

Selecting *Quick Key Definition...* or *Format...* opens the AC Summary Table Format dialog box, where the user defines what information is included in the atomic concentration table when it is generated (AC Summary Table Format on the left side of the dialog box) and what actions are taken when the % button in the upper toolbar is pressed (Quick Key Definition (%)) on the right side of the dialog box).

The left side of the dialog box defines how the atomic concentration table is to be built:

- Information from the data file: included in the header only (Header selected), in the table only (Table selected), or in both the header and the table (Header+Table),
- Information generated by MultiPak when creating the AC table:
  - *Abscissa*—points along the x axis, listed in the first (left-most) column.

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- *Relative Sensitivity Factor*—values from the current database,<sup>2</sup> listed at the top of each column.

*NOTE: The AES sensitivity factors used in the AC calculations on AES data are based on a 5-point differentiation. AES survey and profile data should have a 5-point differentiation applied before performing AC calculations. (No other data reduction should be performed on the data before doing the AC.)*

*NOTE: AC calculations for AES data measured with the 4700TFA or Versaprobe II are performed with corrected sensitivity factors for SCA analyzers. See Appendix A for the correction calculation. Use 0.6% energy resolution data for AC calculations.*

*NOTE: There are two types of the XPS sensitivity factors, one is written as RSF and the other is System RSF. RSFs are the relative sensitivity factors for an instrument with an ideal energy to intensity response function (constant to energy), and assuming the peak intensities proportional to the intensity with whole solid angle of emission. RSF of F 1s determined as unity. The original data were based on Wagner et. al.<sup>3</sup>). Corrected RSFs are the relative sensitivity factors for the instrument used, calculated from the system geometry and transmission parameters stored. Analyzer acceptance angle is ignored to the angular distribution of photoemission.*

- *Concentration*—values in units of percent atomic concentration. When Concentration is selected, the table's title is “Atomic Concentration Table.”

*NOTE: When both Concentration and Intensity are selected, two separate tables with different titles are generated.*

- *Intensity*—values in counts per second. When Intensity is selected, the table's title is “Intensity Table.”
- *Weight %*—concentrations displayed in weight (mass) percent.

*NOTE: When both Concentration and Intensity are selected, two separate tables with different titles are generated.*

- *Mean/Std. Deviation*—mean/standard deviation.

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2 See also AC%; Load; Save As...; Transition Dialog Box; Appendix A, “Atomic Concentration,” “Sensitivity Factors”; Appendices B and C.

3 C.D.Wagner, L.E.Davis, M.V.Zeller, J.A.Taylor, R.H.Raymond and L.H.Gale, *Surface and Interface Analysis*, 3(5), 211 (1981), "Empirical Atomic Sensitivity Factors for Quantitative Analysis by Electron Spectroscopy for Chemical Analysis"

### **3: MultiPak Functions**

- *Tab Delimiter*—tab delimiters added between fields (for pasting into a spreadsheet application).

The right side of the dialog box identifies what functions to execute when the **%** button is pressed in the upper toolbar of the Spectrum or Profile window:

- *Clear*, when on, removes all AC data from the text editor file.
- *Add*, when on, generates AC data and appends it to the data in the text editor file.
- *View*, when on, displays the AC table(s) in the text editor.
- *Print*, when on, sends the table to the printer.
- *Setup*, when on, causes the Atomic Concentration Table dialog box to open.

Pressing **OK** in the Format dialog box saves the settings and closes the dialog box. Pressing **Cancel** closes the box without saving any changes. Pressing **View** displays the table according to the current settings.

*See also AC%; Atomic Concentration; Appendix A, “Atomic Concentration.”*

## **Auto Reduction**

Selecting Auto Reduction from the Tools menu of the Spectrum window performs the actions that are already selected in the current Auto Reduction Setup dialog box for that window. The file name containing the current autoreduction setup is listed in parentheses as part of the menu item (e.g., “Auto Reduction (autored)”).

*See Auto Reduction Setup....*

## **Auto Reduction Log**

All autoreduction operations and errors that occur during an autoreduction sequence are written to a file which can be viewed or printed using Tools–Auto Reduction Log. Each time a new autoreduction sequence is performed, this file is overwritten.

## **Auto Reduction On Open**

When this option in the Open dialog box is turned on, the functions selected in the current autoreduction setup dialog box for that file type are performed automatically when a file is opened.

*NOTE: The processing performed on a file is listed in the third line of the file header.*

*See Auto Reduction Setup...; Open.*

## **Auto Reduction Sequences**

The Auto Reduction Sequences cascading menu lists files having the extension .AUT, which contain permanently saved autoreduction settings. Any of these .AUT files can be executed by selecting a file name from this menu. These files can be edited by starting the *Load...* function in the File menu of the Auto Reduction Setup dialog box and double-clicking on it in the following directory:

*c:\multipak\v9.0\userdata\phiouser1\autored*

*See also Auto Reduction Setup....*

## Auto Reduction Setup...

Selecting the Auto Reduction Setup... function from the Tools menu opens the current autoreduction file (AUTORED.AUT or the last .AUT file that was open), which contains the current Auto Reduction Setup dialog box for that window: Spectrum Autoreduction Setup, Profile Autoreduction Setup, or Map Autoreduction Setup. The settings in the dialog box determine what actions are performed when one of the following actions is taken:

- Auto Reduction is selected from the Tools menu,
- The **Process** button in the Auto Reduction Setup dialog box is pressed,
- A file is opened with Autoreduction On Open turned on in the Open dialog box:
  - *.SPE File(s) opened*—Spectrum Autoreduction Setup dialog is executed after *each* file is loaded in New or Replace mode, or after *all* files are loaded in the Overlay or New/Ovr mode.
  - *.PRO, .ANG, or .LIN file(s) opened*—First, Spectrum Autoreduction Setup dialog is executed and profiles are updated, if Do Spectrum Autoreduction First is selected in the Profile Autoreduction Setup dialog box. Then, the Profile Autoreduction Setup dialog is executed.
  - *.MAP, .ABS, .BSE, .PHO, .SEM, or .SXI file(s) opened*—The Map Autoreduction Setup dialog is executed after all files are loaded.

*NOTE: Many spectrum operations have no effect on map spectra; they only operate on the composite spectrum displayed in MultiPak.*

The order in which MultiPak performs the reduction functions in each setup dialog box is top to bottom.

The dialog boxes are arranged horizontally; that is, parameters to be defined for a function are selected from drop-down menus to the right of and on the same line as the function itself. For example, the Smooth function has two option menus: one for selecting the points to use for smoothing, and the other to specify the type of smooth (e.g., Savitsky-Golay). The option menus sit to the right of and on the same line as “Smooth” in the dialog box.

Settings can be saved permanently in another .AUT file using the dialog box’s File—Save As... function. These files are then listed in the Auto Reduction Sequences cascading menu, and can be executed by selecting one of them from that menu. Files having the extension .AUT can be edited by loading them using the Autoreduction Setup dialog box’s File—Load... function.

Changes in the autoreduction setup dialog box (AUTORED.AUT) are saved by selecting the dialog box’s File—Save menu item, pressing the **Save**

### **3: MultiPak Functions**

button, or pressing the **OK** button. Pressing the **OK** button also closes the dialog box.

Pressing **Process** performs the selected functions. (Note that the processing performed on a file is listed in the third line of the file header.)

**Cancel** closes the dialog box and does not save the settings.

For details about how each function (Smooth, Normalize, etc.) operates, refer to the full description of that function elsewhere in Section 3.

*See also* Auto Reduction Sequences.

## **Axis Properties**

The Axis Properties dialog box is accessed using [Shift]-Left mouse button when pointing at either axis (or a blank area) of the selected data display.

The Axis Properties dialog box allows the user to modify the axes titles and scales of the selected data. Figures 3-4 through 3-7 demonstrate this function. Note that the ranges and names of the x and y axes have been changed in the dialog box and applied to the selected data to demonstrate this capability.

Pressing the **OK** button in the dialog box saves the settings and closes the dialog box. Pressing **Apply** displays the changes without saving the changes. **Cancel** closes the dialog box and does not save the changes.

## **B+W PostScript...**

*See Export To.*

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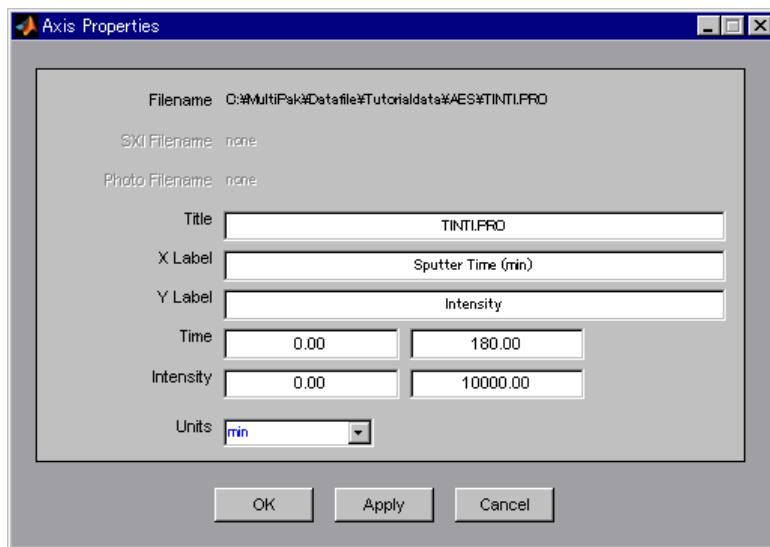


Figure 3-4. Example of an Axis Properties Dialog Box before Revision.

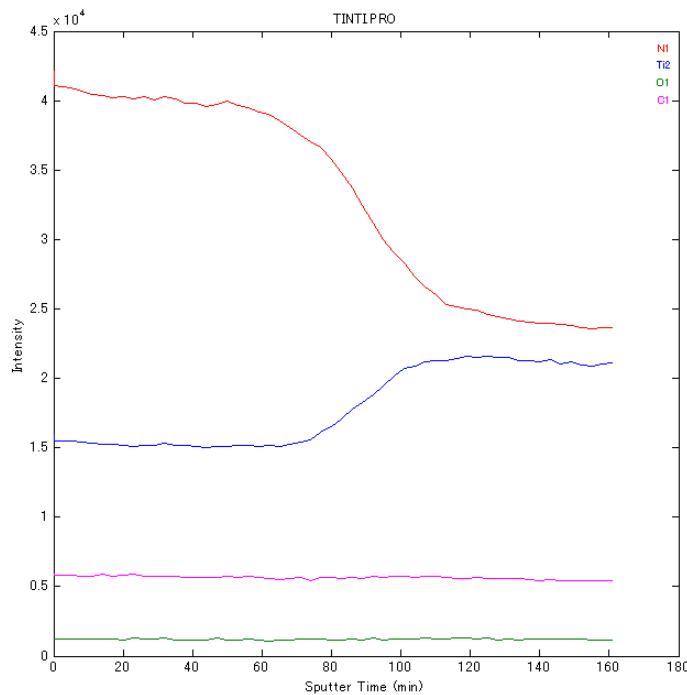


Figure 3-5. Profile Window for Original Axis Properties Dialog Box in Figure 3-4.

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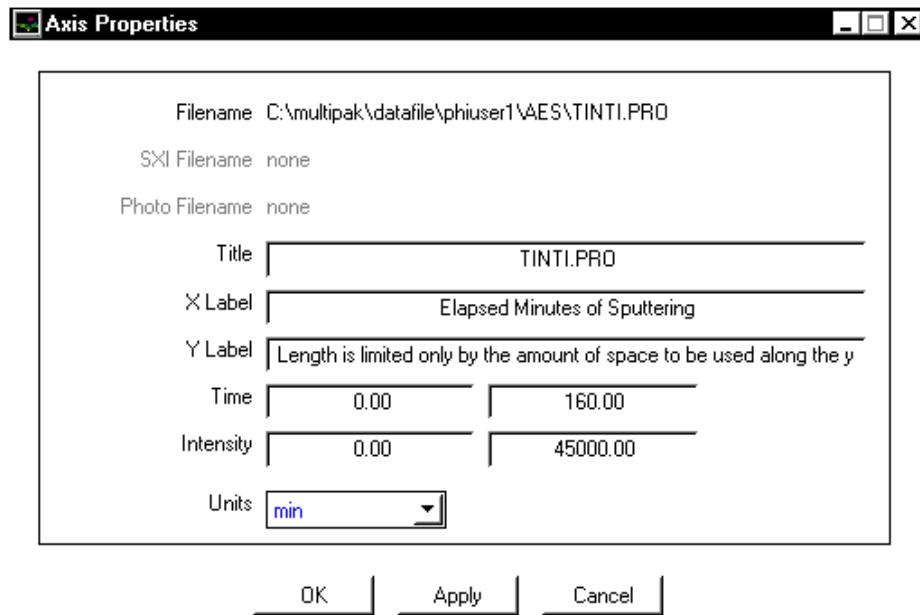


Figure 3-6. Example of an Axis Properties Dialog Box after Revision.

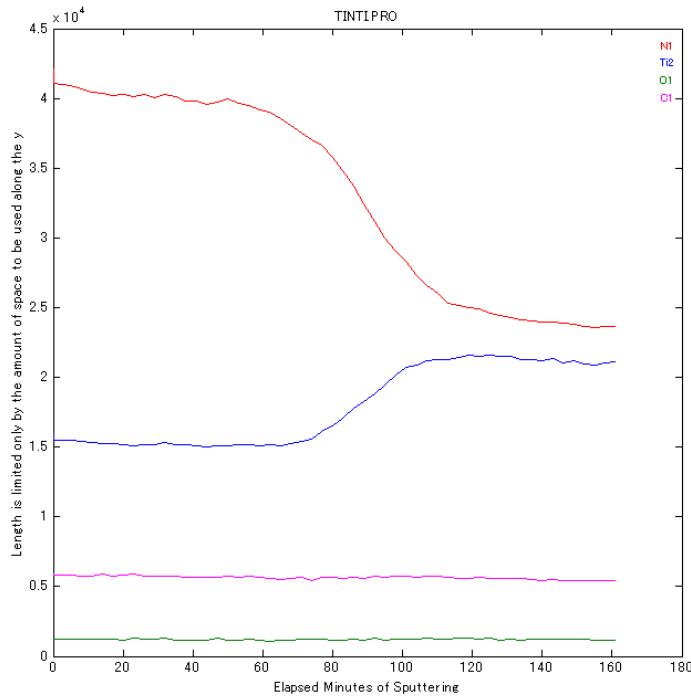


Figure 3-7. Profile Window for Revised Axis Properties Dialog Box in Figure 3-6.

## Background Subtract

The Background Subtract function, found on the Data menu of the Spectrum window, calculates a background curve and subtracts the background curve from the data curve, and displays the data curve with the background

removed. The type (shape) of background curve is selected in the Analysis Region Properties or Transition dialog box.

The Background Subtract (Offset) function, found on the Data menu of the Spectrum window, calculates a background curve, subtracts the background from the data curve, *and displays the background subtracted data curve with its most negative intensity point set to zero (0).*

The Background Subtract (Truncate) function, found on the Data menu of the Spectrum window, calculates a background curve, *subtracts the background from the data curve, sets all negative data points of the result to 0, and displays the adjusted curve.*

*See also* Analysis Region Properties; Transition Dialog Box; Appendix A, “Background.”

## **Background**

*See Appendix A, “Background” and “FWHM/Area....”*

## **Baseline Subtract**

*See Background Subtract.*

## **Beam Size...**

This function operates only on *line* data files (.LIN) in the Profile window. When activated from the Tools menu of the Profile window, it displays the lower toolbar plus six cursors. The operator drags the cursors to measure the spatial resolution (beam size) of a feature in a line scan, as follows:

1. Drag the outer horizontal cursors to the minimum and maximum y values of the data set.
2. Select one of the radio buttons in the lower toolbar (88/12, 84/16, or 80/20). MultiPak automatically positions the middle two horizontal cursors based upon this selection.
3. Drag the left and right vertical cursors so they align with each intersection of the data and the two middle horizontal cursors. Beam size, in the units of the x axis, will be displayed automatically on the right side of the lower toolbar.

Click on **DispAll** to select another element profile for analysis of beam size. Pressing **Exit** closes the Beam Size toolbar.

## **Bin3**

*See Smooth (Binomial 3); Smooth/Derivative Setup....*

## **Black**

*See Annotate...; Color Option Menu; Data Properties.*

## **Blue**

*See Annotate...; Color Option Menu; Data Properties.*

## **Bold**

*See Annotate....*

## **Calculate...**

*See Intensity Calibration.*

## Chemical State ID...

Selecting Tools—Chemical State ID... in the ESCA Spectrum window zooms to the first region defined, places an energy cursor at the peak energy defined in the peak identification database for the region, places the selection slider and buttons in the Spectrum window, and displays the Chemical State Identification dialog box listing possible chemical states from MultiPak’s XPS database for the region, transition, “identification” (binding) energy, and specified energy range. The chemical state whose energy is closest to the current identification energy will be highlighted in the list automatically.

The user can select one spectrum or a set of contiguous or noncontiguous spectra to use for the routine using the selection slider. The energy cursor can be dragged and released to display all possible chemical states for a different energy. Typing different values into the Identification Energy or Energy Range fields and pressing Enter on the keyboard also changes the display of chemical states.

One or more chemical states can be selected from the list using the mouse button alone or with the Shift or Ctrl keys for multiple selections. Pressing the **Annotate** button in the dialog box adds the name(s) of the selected chemical state(s) to the current spectra at the location of the identification energy.

Pressing **Delete** removes all Chemical State ID annotation from the current spectra. Pressing **Exit** closes the dialog box, saving the current value in the Energy Range field.

Pressing **Database** displays the Chemical ID Database dialog box to edit the database. Selecting the target chemical state in combo-box and then pressing Delete to delete the selected chemical state item. Pressing **Add** appends the displayed chemical state to the database. The revised database is applied to the original database by pressing Write Database or OK button.

Selecting Edit—Clear Annotation—Chemical State ID removes any Chemical State ID-style annotation from the current data.

*See also Annotate...; Energy Cursor; Select Spectra...; Appendix B, “XPS Sensitivity Factors.”*

## Clear

*See Atomic Concentration Table; Periodic Table.*

## **Clear All**

For a description of the operation of this button, refer to the function with which it is associated.

## **Clear All Annotation**

Selecting Clear All Annotation on the Edit menu deletes all annotation from the current (selected) data, including annotation that is not currently displayed due to expansion etc. Pressing the **Clear All** button on the lower toolbar during the Annotate... function does the same thing.

*See also* Clear Annotation.

## **Clear Annotation**

Selecting an item from the Edit–Clear Annotation submenu deletes the selected annotation type from the current data: *Text*, *Peak ID* labels, *Chemical State ID* labels, *Tables*, *Fingerprint*, *Legend*, or *Markers*. For example, peak labels that are added to data using the Peak ID function are associated with the “Peak ID” type of annotation. Selecting Edit–Clear–Peak ID removes peak labels added using the Peak ID function.

*See also* Annotate...; Clear All Annotation; Labels Option Menu.

## **Close**

Selecting Close from the File menu of any MultiPak window closes the file currently selected *in that window*. (The name of the currently selected file is displayed in two places: (1) in green directly above the selected data, and (2) in the status bar at the bottom of the window.)

All displays of that file will be removed from the MultiPak windows. (The original data acquisition file is not changed, and no MultiPak windows will be closed.)

*See also* Close All; Exit; Close and ReOpen.

## **Close All**

Selecting Close All from any MultiPak File menu closes all open MultiPak files.

(Switching from ESCA to AES or AES to ESCA in the File–Options menu also closes all MultiPak files currently open.)

*See also* Close; Exit; Close and ReOpen.

## **Close and ReOpen**

Close and ReOpen is available on the File menu. Selecting this function causes the currently selected file in that window to close and reopen. This is a quick way of reverting back to the original acquisition data before trying a different data reduction function.

## Color Bar

The color of an image in the Map window is determined first by the selection in the color option menu, but also by the settings of the color bar to the right side of each image.<sup>4</sup> Table 3-2 summarizes the mouse functions available on the color bar. (Refer to the maps in the tutorials in Section 2 for illustrations of the color bar.)

The color bar has three sliding handles. The left one can be dragged with the mouse to change the *brightness*, or Gamma, of the displayed image. The two right handles can be dragged up and down to adjust the *contrast* or the *threshold*, depending on which mouse buttons are used. The settings can also be adjusted by manually changing the settings values in the Color Bar Properties dialog box, which is displayed by [Shift]-left clicking on the color bar.

The number at the top of the color bar is the maximum number of counts per second (or percent concentration if the AC% box is checked in the upper toolbar); the bottom number is the minimum. These values will change when the contrast is changed.

In a contrast operation, the new position(s) of the handle(s) define a new range of contrast, and every pixel in the image is assigned a new contrast value accordingly. The threshold operation removes (sets to zero) all data values outside the threshold limits, which does not visibly change the color bar.

Table 3-2. Mouse Functions during the Color Bar Function.

To:	Point At:	Press:
Adjust the brightness of the displayed image	left handle	Left and drag
Adjust the upper value of contrast used for display	1. closed top right handle 2. open top right handle	1. Left and drag 2. Right
Adjust the lower value of contrast used for display	1. closed bottom right handle 2. open bottom right handle	1. Left and drag 2. Right
Adjust the threshold used for display	1. closed right handle 2. open right handle	1. [Shift]-left & drag 2. Right
Cancel the contrast or threshold operation before resolving it	open right handle	Left and drag the handle back to and beyond its original

4 NOTE: The colors used to display a map are also determined by whether one or more maps are displayed in the window. When one map is displayed, 128 colors are used; when more than one map is displayed, only 24 colors are used for each map.

		location at the top or bottom of the color bar
--	--	--

To improve the quality of an image, start by using the left mouse button to drag the lower contrast handle, on the right side of the color bar, upward to create more uniform black areas, then click on the open handle with the right mouse button to resolve it. Then, use the left mouse button again to drag the upper contrast handle downward to create more uniform colored areas, then click on the open handle with the right mouse button to resolve it. Continue, if needed, in the same way until you achieve the desired image and contrast quality.

When changing these values using the Color Bar Properties dialog box and pressing the **Apply** or **Apply All** button, the threshold operation is performed first, followed by the contrast operation.

*NOTE: Selecting contrast and/or threshold values greater than those currently entered is allowed. Selecting contrast values beyond the data limits is also allowed and darkens the image. Selecting threshold values beyond the data limits will have no effect on the data.*

Pressing the **Apply** button displays the results of the current settings. Pressing the **OK** button applies the changes to the current image and closes the dialog box. **Cancel** makes no changes and closes the dialog box, except those made if **Apply All** was pressed in the dialog box. The **Apply All** button changes the settings of all map images.

To restore the current image to the default brightness, contrast, and threshold; press the **Default** button. To restore all images to their defaults, press the **Default All** button.

*See also* Color Option Menu.

## **Color Bar Properties**

*See* Color Bar.

## **Color Option Menu**

The color option menu is available in the lower toolbar of the Map window. The setting of this menu determines the colors used to display the image. The menu items include gray, thermal, pseudo, red, green, blue, pseudo2, pseudo3, yellow, cyan and magenta. The colors associated with each menu choice are shown in the color bar to the right of the image.

*NOTE: The colors used to display a map are also determined by whether one or more maps are displayed in the window. When one map is displayed, 128 colors are used; when more than one map is displayed, only 24 colors are used for each map.*

*See also* Color Bar.

## **Color PostScript...**

*See* Export To.

## **Compare...**

The Compare... function, available from the Data menu of the Map window, displays a lower toolbar. Compare performs a comparison between two or more images. One image becomes the reference image to which the other images are compared. The images to be compared can be divided (pixel by pixel) by the reference image or have the reference image subtracted from them.

The reference image has its title set to brown. Clicking on a map makes it the reference image. Clicking on /Ref causes the other image(s) to be divided by the reference image, and the resulting data is displayed in place of the other image(s). Clicking on -Ref causes the other image(s) to be replaced by that image minus the reference image.

Only images with the same x and y dimensions can be compared.

*See also* Add/Subtract/Compare....

## **Contrast**

*See* Color Bar.

## **Copy To Clipboard**

The Copy To Clipboard function may be selected from the Edit menu of any MultiPak window.

Copy To Clipboard writes the contents of the current window (only the display of the header and data) to the clipboard for pasting into files of other applications.

Copy To Clipboard(Bitmap) writes the contents of the current window to the clipboard as bitmap format.

Copy To Clipboard(Custom) writes the contents of the current window to the clipboard with setting set in the Copy To Clipboard Setup... and without space blank.

### **3: MultiPak Functions**

When activated the Copy To Clipboard Setup... the Copy To Clipboard Setting windows is displayed. In this window, operator can select show/not show header, magnification ratio of pasted window, magnification ratio of header font size, magnification ratio of graph font size, anti-aliasing. Pressing OK apply settings and closes Copy To Clipboard Setting window.

- Header : Select whether the header is included to the paste contents or not.
- Canvas Scale : Select the magnification ratio of pasted window. When the pasted windows size is more than monitor resolution, this parameter is adjusted automatically.
- Header Font Scale : Select the magnification ratio of header font size.
- Graph Font Scale : Select the magnification ratio of graph font size.
- Anti-Aliasing : This option prevented the border or slant line of pasted image to be stepwise. This option can be set each window.

## **Courier New**

*See Annotate....*

## **Create/Update Map**

*See Imag/New.*

## **Cursor**

*See Region Cursors; Energy Cursor.*

## **Curve Fit...**

This function is started from the Tools menu or the Fit button in the upper toolbar of the Spectrum window. The Curve Fit routine is performed on the selected spectra within the selected energy region when the **Fit** button in the lower toolbar is pressed.

The Curve Fit routine in MultiPak provides the ability to define synthetic bands (curves) underneath the data curve in order to isolate multiple chemical species that may be present. The routine provides access to a number of parameters that can be used to define the synthetic bands including: band shape (i.e., peak shape) options (Gaussian, Gaussian-Lorentzian, and Asymmetric Gaussian-Lorentzian), multiplet locking options (band separation locking and band area ratio locking), parameter limit settings, background correction options (linear, Shirley, iterative Shirley, and none), interactive initialization of band parameters, FWHM locking, and the option to redefine and turn on/off the default parameter limits.

### **3: MultiPak Functions**

With this routine, the user can develop a synthetic peak structure that is composed of a number of peaks of a standard type, superimpose this peak structure data set, and adjust the parameters defining the synthetic peak structure to simulate the acquired spectral data. This can help the user to more effectively identify chemical states and quantify them.

Table 3-3 shows some of the Curve Fit mouse functions.

*Table 3-3. Mouse Functions in Curve Fit.*

To:	Point At:	Press:
Create a new band	highest point of the desired peak location	Right
Adjust height or position	top handle of synthetic curve	Left & drag on handle
Adjust width	right-hand handle of synthetic curve	Left & drag on handle
Adjust asymmetric tail	left-hand handle of synthetic curve	Left & drag on left-hand handle
Select an existing band	synthetic curve	Left

### **Curve Fit Toolbar Buttons**

The buttons in the toolbar change depending upon whether the **Setup** check box in the lower toolbar of the Spectrum window is checked or not. When the **Setup** check box is checked, the Curve Fit function is in setup mode. When the Setup check box is unchecked, the Curve Fit function is in batch fit mode.

When the **Fit** button is pressed, the curve fit is performed on the spectrum. Any parameter in the Curve Fit Setup dialog box that has reached a limit during the fitting process will be displayed in red.

The **PrevBand** and **NextBand** buttons change the current band (the one displayed with adjustment handles). **DelBand** and **DelAll** delete the current band or all bands. These buttons are available in the setup mode only.

**ShowAll** displays all spectra (in a depth profile, for example), and **ShowOne** displays one spectrum and its component spectra (bands) from the fitting. Use the left mouse button to move the spectra selection slider to display another spectrum and its component spectra, or to select a different range of the spectra to be displayed. These are available only in the batch fit mode except for map curve fit.

**MeanSpec** displays mean spectra, and **SelectArea** displays selected spectra which are extracted from a map and their component spectra from the fitting. Use the left mouse button to select anywhere on the map display. These functions are available only in the batch fit mode and only for maps.

Pressing the **Prof/New** (or **Map/New**) button generates a profile for each band after fitting a group of spectra (e.g., a depth profile data set). This is available only in the batch fit mode.

The **New** check box, when checked, overwrites the Summary Table file with the new curve fit results on each fit. The **SumSetup** button displays the Curve Fit Summary Table Setup dialog box to allow customization of the summary table. The **ViewSum** button displays the current Curve Fit Summary Table in a Notepad window. The **PrintSum** button prints the current Curve Fit Summary Table.

The **Append** button (available only when the **New** check box is not on) adds the current curve fit results to the previous Curve Fit Summary Table. The **ClearSum** button (available only when the **New** check box is not on) clears the current Curve Fit Summary Table.

The **Exit** button exits the Curve Fit application. This button is available in both the setup and batch fit modes.

### **3: MultiPak Functions**

When clicking the **SelectArea** button, refresh the Map window to the select area mode.

The **Polygon** radio button allows any complex area to be drawn on the map.  
The **Rectangle** radio button allows a rectangular area to be drawn on the map.

The **Cut** button will delete the currently selected area.

The **ViewSpc** button generates a spectrum and associated band peak in the Spectrum window. This is available only in the select area mode.

### 3: MultiPak Functions

Table 3-4. Lower Toolbar Function during Curve fit

<b>Setup mode only</b>		
<b>Button / Check box:</b>	<b>Function:</b>	<b>Note:</b>
Fit	curve fit is performed on the spectrum.	Any parameter in the Curve Fit Setup dialog box that has reached a limit during the fitting process will be displayed in red.
PrevBand and NextBand	change the current band (the one displayed with adjustment handles).	
DelBand and DelAll	delete the current band or all bands.	
<b>Batch fit mode only (except for map curvefit)</b>		
ShowAll	Display all spectra (in a depth profile, for example)	
ShowOne	display one spectrum and its component spectra (bands) from the fitting.	Use the left mouse button to move the spectra selection slider to display another spectrum and its component spectra, or to select a different range of the spectra to be displayed.
Prof/New	Generate a profile for each band after fitting a group of spectra (e.g., a depth profile data set).	
<b>Batch fit mode only (for map curvefit)</b>		
MeanSpec	display the mean spectrum of all pixels in the map.	
SelectArea	display the Map window to define areas on the map.	Use the left mouse button to select anywhere on the map display.
Map/New	generate a maps for each band after fitting a group of spectra (e.g., a map data set).	
<b>For summary table</b>		
New	when checked, overwrites the Summary Table file with the new curve fit results on each fit.	
SumSetup	display the Curve Fit Summary Table Setup dialog box to allow customization of the summary table.	
ViewSum	display the current Curve Fit Summary Table in a Notepad window.	
PrintSum	print the current Curve Fit Summary Table.	
Append	add the current curve fit results to the previous Curve Fit Summary Table. (available only when the <b>New</b> check box is unchecked)	
ClearSum	clear the current Curve Fit Summary Table (available only when the <b>New</b> check box is unchecked).	
<b>Select area mode (for map curvefit)</b>		
Polygon radio button	allow the drawing of any complex area on the map.	
Rectangle radio button	allow the drawing of a rectangular area on the map.	
Cut	delete the currently selected area.	
ViewSpc	generate a spectrum and associated band peak in the Spectrum window	

**Procedure**

To perform a curve fit on spectral data, do the following:

1. Select the peak and energy range of interest using region buttons and the analysis region cursors. If the spectrum has no region buttons associated with it, create them using the Periodic Table.
2. Perform any necessary data reductions, such as smoothing or shift.
3. If the data set contains more than one spectrum (e.g., multiple analysis points, depth profiles) in the selected energy range, you will need to select which spectrum or group of spectra will be fit. If no selection is made, all spectra in the selected energy range will be fit.
4. Press the **Fit** button in the upper toolbar to start the function.

The background is drawn on the spectral display (unless None is specified in the Analysis Region Properties or Transition dialog box as the background type), and the Curve Fit Setup dialog box is opened. (The background type initially applied is determined by the background type specified in the Analysis Region Properties or Transition dialog box.)

5. Check the **Setup** check box in the lower toolbar, if it is not already checked. If more than one spectrum has been selected for curve fitting, a composite peak will be displayed.
6. In the Curve Fit Setup box, select the peak shape type. (A Gaussian-Lorentzian peak shape is used in most cases.)

### **3: MultiPak Functions**

7. Using the right mouse button, click at the top of the most intense peak of the data set, then drag. This creates the first band to be used in the fit.

A synthetic curve is displayed, plus a red dashed line below the baseline. The red dashed line represents the difference (error) between the synthetic curves and the original data.

8. If desired, adjust the peak shape by dragging the curve's handles (small boxes on the peak and the same color as the peak) with the left mouse button. Peak shape and position may also be changed by manually entering numbers in the Setup box.
9. Repeat steps 6 through 8 to create bands for the remaining peaks.
10. Press the **Fit** button in the lower toolbar of the Spectrum window to perform a nonlinear least squares fit (curve fit).

The new synthetic curves and error curve are displayed. The fields of the setup dialog box are updated; those that display red parameters after performing the fit indicate that the limits for that parameter were reached. Limits are defined in the Band Limits dialog box.

*NOTE: A red parameter value is acceptable, indicating only that it is at its currently defined limit. The user needs to evaluate the appropriateness of each parameter value, changing values only as needed.*

After evaluating the curve fit results, changes may be made by entering new values in the Curve Fit Setup box fields or by selecting a band with the left mouse button and adjusting its position or shape by grabbing and dragging the handles on the band.

Spectra from reference samples or ESCA databases, such as the PHI *Handbook of X-ray Photoelectron Spectroscopy*\* or the NIST XPS database, may be used to evaluate the curve fit results. It is possible to generate a mathematically correct result that makes no chemical sense. For this reason, curve fitting results should be carefully evaluated by the user.

Press the **Fit** button in the lower toolbar again if changes have been made in the **Setup** check box. Repeat steps 10 and 11 until satisfactory results are obtained.

11. When the fit is satisfactory, click on the **Setup** check box in the lower toolbar of the Spectrum window to switch to the batch ft mode.

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\* John F. Moulder et al., *Handbook of X-ray Photoelectron Spectroscopy*, Eden Prairie: Physical Electronics, (1995).

12. If multiple spectra were originally selected for curve fitting, press **Fit** in the lower toolbar to apply the fit parameters to all the spectra.
13. If multiple spectra were curve fit, press the **Prof/Upd** button in the lower toolbar of the Spectrum window to create, in the Profile window, a series of chemical profiles that contains the curve fit results.
14. When finished, press **Exit** in the lower toolbar of the Spectrum window to end the curve fit routine.

To perform a curve fit on map data, do the following:

1. Select the peak and energy range of interest using region buttons and the analysis region cursors as for fitting spectral data above.
2. Press the Fit button in the upper toolbar to start the function.

The background is drawn on the spectral display (unless None is specified in the Analysis Region Properties or Transition dialog box), and the Curve Fit Setup dialog box is opened. (The background type initially applied is determined by the background type specified in the Analysis Region Properties or Transition dialog box.)

3. Uncheck the **Setup** check box in the lower toolbar. Press the **MeanSpc** button in the lower toolbar of the Spectrum window to display the mean spectrum of all pixels in the map. Press the **SelectArea** button in the lower toolbar of the Spectrum window to display the Map window to define areas on the map; the spectrum from these areas will be used for curve fit setup.
4. Click and drag the mouse using the left button to define a rectangular or polygonal area on the map. Polygons of any complexity may be drawn. To create a side, click, drag, and release the left mouse button. To close the polygon, click and release the left mouse button without moving the mouse: The software fills in the last side of the polygon, so it is not necessary to join the endpoints manually.
5. Press the **ViewSpc** button in the lower toolbar of the Map window to display a spectrum from the defined area in the Spectrum window. If the **Overlay** check box in the lower toolbar of the Map window is checked, the total area spectrum is overlaid with those for all selected areas on the map. If it is unchecked, the new spectrum is averaged with all selected areas.
6. Check the **Setup** check box in the lower toolbar, if it is not already checked. If more than one spectrum has been selected for curve fitting, a composite peak will be displayed. In the Curve Fit Setup box, select

### **3: MultiPak Functions**

the peak shape type. (A Gaussian-Lorentzian peak shape is used in most cases.)

7. Using the right mouse button, click at the top of the most intense peak of the data set, then drag. This creates the first band to be used in the fit.

A synthetic curve is displayed, plus a red dashed line below the baseline. The red dashed line represents the difference (error) between the (composite) synthetic spectrum and the original data.

8. If desired, adjust the peak shape by dragging the curve's handles (small boxes on the peak and the same color as the peak) with the left mouse button. Peak shape and position may also be changed by manually entering numbers in the Setup box.
9. Repeat steps 8 through 9 to create bands for the remaining peaks.
10. Press the **Fit** button in the lower toolbar of the Spectrum window to perform the nonlinear least squares fit (curve fit).

The new synthetic curves and error curve are displayed. The fields of the setup dialog box are updated; those that display red parameters after performing the fit indicate that the limits for that parameter were reached. Limits are defined in the Band Limits dialog box.

*NOTE: A red parameter value is acceptable, indicating only that it is at its currently defined limit. The user needs to evaluate the appropriateness of each parameter value, changing values only as needed.*

### **3: MultiPak Functions**

After evaluating the curve fit results, changes may be made by entering new values in the Curve Fit Setup box fields or by selecting a band with the left mouse button and adjusting its position or shape by grabbing and dragging the handles on the band.

Spectra from reference samples or ESCA databases, such as the PHI Handbook of X-ray Photoelectron Spectroscopy\* or the NIST XPS database, may be used to evaluate the curve fit results. It is possible to generate a mathematically correct result that makes no chemical sense. For this reason, curve fitting results should be carefully evaluated by the user.

Press the **Fit** button in the lower toolbar again if changes have been made in the Setup box. Repeat steps 10 and 11 until satisfactory results are obtained.

11. When the fit is satisfactory, click on the Setup check box in the lower toolbar of the Spectrum window to switch to the Batch Fit mode.
12. If multiple spectra were originally selected for curve fitting, press **Fit** button in the lower toolbar to apply the fit parameters to all the spectra.
13. If multiple spectra were curve fit, press the **Map/Upd** button in the lower toolbar of the Spectrum window to create, in the map window, an image of chemical map that contains the curve fit results.
14. When finished, press **Exit** in the lower toolbar of the Spectrum window to end the curve fit routine.

### **Curve Fit Setup Dialog Box**

The Curve Fit Setup dialog box (shown in Section 2) defines the band parameters that determine the shape of the synthetic curves (bands) to be used for fitting. The File menu of this dialog box is used to create and load band setup files for reuse on other files. The dialog box has three parts, described as follows.

#### **File Menu in the Setup Dialog Box**

The File menu has Open... and Save and Save As... and Save Result... options. Open is used to specify a file name that contains previously defined band settings to be used on all bands in the data file. Save and Save As... are used to store the current band settings to be used on other files. Save Result... is used to store all of the bands, spectra, the raw spectrum, the background spectrum, and the error spectrum. These files are stored with a common root name. If spectrum files are used, the saved files are .SPE extension. If profile files are, the saved files are .PRO extension. The Export To button is used to save all of the curvefit bands as CSV format file. When the *Row* option is selected in the System Constants dialog box for “ASCII Format”, the blocks are ordered horizontally. If *Column* option is selected, the blocks are arranged vertically. The System Constants dialog box is accessed from the following path: File/Options/System Settings.

#### **Setup Menu in the Setup Dialog Box**

The Setup menu has Summary Table..., Annotation..., Doublet...and Chemical State ID... options. Summary Table is used to open the dialog box to customize a summary table. This option is same as “SummSetup” button. Annotation is used to open the dialog box to customize an annotation table that user paste on the graph. Doublet is used to open the dialog box to the dialog box to edit the doublet band database. Chemical State ID is used to open the dialog box to select the chemical state from the peripheral information which is selected by both the active band position and the Chemical State ID database.

#### **Annotation Setup Dialog Box**

The Annotation Setup dialog box has BandName, ChemicalState, Position, Separation and Area checkbox options. User can customize an annotation table using checking each checkbox options. Press the OK button to apply the current setting. Press the Annotate button to paste an annotation table on the graph. Press the Reset button to load the initial setting.

### ***Doublet Setup Dialog Box***

The Doublet Setup dialog box has Element, Peak Separation, Area Ratio and Label edit options. User can select the element in the Element combo-box option to edit band properties to be pair. Press the New button to register the new element. Press the Delete button to delete the current element from the database. Pressing the OK button, the current setting is applied.

### ***Chemical State ID Setup Dialog Box***

Chemical State ID Setup dialog box lists the chemical state information which is peripheral chemical position and chemical name of the current band's position. Press the Apply button to apply the chemical state label on the "Chem State" parameter of the current band.

### ***Top of the Setup Dialog Box***

The top of the Curve Fit Setup dialog box has the following elements:

- Max Iterations is used to specify the maximum number of fitting iterations applied to the spectrum.
- The band (peak shape) list box specifies the mathematical function(s) used to define the peak shapes of the synthetic curves (bands): Gauss, Gauss-Lorentzian, or Asymmetric Gauss-Lorentzian.
- The background-type list box allows you to specify the type of background subtraction (Shirley, Iterated Shirley, Linear, or None) to perform on all spectra before the fitting process. (Refer to Appendix A, "Background" for definitions of these background types.)
- ChiSquared displays the  $\chi^2$  value for fitting each spectrum. A small value for  $\chi^2$  indicates a good fit.
- A message field for display during the fitting process.

### ***Middle of the Setup Dialog Box***

The middle of the Setup dialog box is where peak-shape, position-locking, and area-ratio-locking parameters may be viewed or changed. The peak-shape parameters are updated automatically when the band handles are dragged to new positions. The values of these parameters can also be specified by the user by double-clicking in the parameter field and typing a new value. The peak-shape parameters are defined as follows:

- *Chem State*—user-defined string for chemical state information;

### 3: MultiPak Functions

- *Area*—area under the peak in that band (calculated by the software and displayed automatically);
- *Band FWHM*—width of the band at one half its height, in eV;
- *Position*—energy of the peak's center, in eV;
- *Height*—height of the peak at the peak's center, in counts;
- *FWHM*—width of the peak component at one half its height, in eV;
- *%Gauss*—mix of Gaussian and Lorentzian contributions to the peak shape, with 0% being a pure Lorentzian curve and 100% being a pure Gaussian curve;
- *Tail Length*—distance, in half width at half maximum, at which the tail becomes insignificant (less than 1% of the height);
- *Tail Scale*—increases or decrease the intensity of the tail shape that is defined by the Tail Length.

*NOTE: Tail Length and Tail Scale are adjusted by the synthetic curve's handle on the left (higher binding energy) side.*

A curve is defined by the Position, Height, and Gauss FWHM parameters. A Gaussian-Lorentzian curve is defined by the same three parameters plus the %Gauss parameter. An Asymmetric Gaussian-Lorentzian combination curve is defined by these four parameters plus the *Tail Length* and *Tail Scale* parameters.

The analyst may define certain bands to be dependent upon other bands. There are three types of dependencies: position locking (fixing the energy separation between two or more bands), area locking (fixing the area ratio between two or more bands), and FWHM locking:

- In position locking (*Lock Pos* and *Separation* parameters), the dependent peak's position is anchored to the independent peak's position by an energy separation. As the independent peak's position is adjusted, the dependent peak's position is also adjusted to maintain this constant separation. For example, to lock the position of band 2 to that of band 1, enter 1 in the Lock Pos field under band 2 and specify the separation in eV in the Separation field under band 2.
- In area locking (*Lock Area* and *Area Ratio* parameters), the dependent peak's area is anchored to the independent peak's area by an area ratio. As the independent peak is adjusted, the dependent peak is also adjusted to maintain the ratio between the areas of the two peaks. For example, to lock the area ratio of band 2 to that of band 1, enter 1 in the Lock Area field under band 2 and specify the area ratio in the Area Ratio field under band 2.
- In FWHM locking, the FWHM Lock parameter is the reference band number to which the FWHM of the current band is locked, and the

### **3: MultiPak Functions**

FWHM Difference parameter is the difference between the current band and the reference band.

*NOTE: Multiple locks (e.g., band 3 to band 2 to band 1) are permitted, but circular locks (e.g., band 2 to band 1 to band 2) are not.*

#### ***Bottom of the Setup Dialog Box***

At the bottom of the Setup dialog box is the band-selection list box, which allows you to select the current band. The **Band Limits...** button opens the Band Limits dialog box. The **Change Default Limits...** button opens the Default Parameters Limits dialog box. The **Apply Default Limits** button applies the current values in the Default Parameters Limits dialog box to either the current band (**Apply to One Band**) or all bands (**Apply to All Bands**), depending on the setting of the option menu next to this button.

*NOTE: The **Apply Default Limits** button must be pressed to impose the default limits on all parameters for the current band.*

#### ***Summary Table Setup Dialog Box***

Pressing the **SumSetup** button in Curve Fit's lower toolbar opens the Summary Table Setup Dialog Box. Here, the user defines how the curve fit results will be written to the system editor application for viewing and printing.

Use the Description Text check boxes to specify whether to put the file information and/or column headers in the next summary. Select one of the Band List radio buttons to specify whether to list data in rows or in columns. Use the Curve Fit Parameters check boxes to specify which band parameters to list in the summary. Select one of the column delimiter radio buttons to specify whether to use a space or tab character as the delimiter character between columns in the summary file.

Pressing the **ViewSum** button displays the Summary Table in a Notepad window according to the selections made in the dialog box. The **Reset** button resets the dialog box settings to default PHI settings.

Pressing **Cancel** discards the current summary table format and closes the dialog box. The **OK** button saves the current summary table format and closes the dialog box.

#### ***Default Parameter Limits Dialog Box***

The default limits are expressed as the differences between the upper and lower limits with half of the difference used symmetrically around the current band parameter values during curve fit processing. The default limits are shared by all bands in a given region, but are saved separately for each region. (All upper and lower limits are checked for non-physical values and adjusted properly to make them physically meaningful.) The set

of defaults is stored in a file named for the region and having the extension “.FIT.” (The original installed defaults are stored in a separate file.)

The default limits for height are fixed at zero for the lower limit and twice the maximum spectra intensity for the upper limit. This is necessary for an efficient batch fitting where peak heights may vary considerably from one spectrum to another spectrum.

The **Close** button closes the Default Parameter Limits dialog box and saves the changes for the current region. The **Save As Global...** button allows saving changes in the default limits to be used as the default for all regions. The **Reset to Global** button resets the limits to the global defaults. This scheme gives the user an easy way to choose different default limits for each region or use the same default limits for all regions.

#### **Band Limits Dialog Box**

The Band Limits dialog box is displayed by pressing the Band Limits button in the Curve Fit Setup dialog box. This dialog box allows changing band limits for each band individually. Any changes made to an individual band in this manner will not be overridden unless the **Apply Default Limits** button is applied to this band.

This dialog box also allows fixing a parameter for part or all of the curve fitting process. The Invariance parameter is used to lock the parameter value to its estimated value for the specified number of iterations. The Fix check box, when on, fixes the band parameter value at the displayed value during the entire curve fit process.

When a parameter is changed in the Curve Fit Setup box, the range (upper and lower) limits are automatically adjusted.

The **Close** button closes the Band Limits dialog box and saves the changes for the current region. The **Save As Default** button saves the differences between the upper and lower limits as default limits for this region.

*NOTE: %Gauss parameter limits of 65 and 50 are typical for a metallic peak.*

## **Cyan**

*See Annotate...; Data Properties.*

## **Cycle Number**

*See Legend.*

## **Data**

The Data menu contains functions that modify the data. In most cases it is possible to save the modified data, however the original data file is always

preserved. The functions in this menu vary with the technique (AES or XPS) and type of data being processed.

## Data Link

The Data Link check box in the lower toolbar of the three main windows, when on, causes linked data in another MultiPak main window to be updated automatically when changes are made to the data displayed in another window, termed the “source” data.

Turning the Data Link check box off can save the time it takes to refresh the display of the linked data in the other window. The display can be refreshed at any time by pressing the **Upd** button in the lower toolbar. The Data Link check box can be turned off and on according to the needs of the analyst.

*NOTE: Data in different windows are linked by pressing the **Spec/New**, **Imag/New**, **Prof/New**, or **Line/New** button in the lower toolbar, with the following exceptions. Data in the Profile window are automatically linked to data in the Spectrum window when a PRO file is opened, and data in the Map window are automatically linked to data in the Spectrum window when an ESCA MAP file is opened.*

*When the data link is in effect, this button is named **Spec/Upd** (update), **Imag/Upd**, **Prof/Upd**, or **Line/Upd**. The button will be named Upd until different data are selected in the source window or another function is activated that breaks the direct link.*

*Pressing the Upd button does manually what turning on the Data Link button does automatically: It assures the user that the linked data reflects the changes in the source data.*

*See also Imag/New; Line/New; Prof/New; Spec/New.*

## Data Parameters

Selecting this function from the File menu displays a cascading menu of two functions. *View* displays the parameters from the current file in a text editor, as shown in Figure 3-8. *Print* prints a hard copy of the parameters last viewed.

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```
Datafile C:\multipak\datafile\phiiuuser1\AES\TINTI.PRO created 96 6 11

Dataset: AES DEPTHPRO
Original datafile: tinti.pro acquired 96 6 11 by user wfs
Instrument model: PHI-ACCESS
File description: TiN/Ti

EBeam source: 1486.6 at 20.00 W
Beam diameter: 10.0 um
Analyser mode: FAT

Sputter source: 5.00 keV Ar+ 200.0 nA
Presputter cycles: 0
Sputter cycles: 55
Sputter mode: alt
Sample rotation: off

-----
Spectral Region Definitions
-----

No Transition Start (eV) End (eV) Inc (eV) Time/DataPt (s)
4 C1 250.00 285.00 0.50 1.000
3 O1 490.00 525.00 0.50 1.000
2 Ti2 400.00 435.00 0.50 1.000
1 N1 365.00 400.00 0.50 1.000
```

Figure 3-8. Display of Data Parameters in a Notepad window.

## Data Properties

The Data Properties dialog box is displayed using [Shift]-left mouse button when pointing at data.

The Data Properties dialog box lets the user change the comments displayed in the header, the scale factor for the data curve, the color, line width, and line style associated with the data.

For spectrum files, the Data Properties dialog box provides the choice to apply the changes to the currently displayed data by selecting **Spectrum** or to apply the changes to all data associated with the current point or area by selecting **Area**.

## Depth

The field on the right side of the lower toolbar of the Profile window displays Depth or Time when the window is active. The window is made active by clicking with the left mouse button on the file name above the data.

The field displays the x-axis value of the location of the mouse pointer. The x-axis value is updated continuously as the mouse pointer is moved back and forth across the depth profile display.

*See also* Intensity.

## **Depth Calibrate...**

The Depth Calibrate... function, available from the Tools menu of the Profile window, is used to adjust the depth scale by defining etch rates for regions of the profile with different sputtering conditions or materials with different etch rates. Selecting Depth Calibrate... opens the Depth Calibrate dialog box and a lower toolbar.

If the selected file has depth calibrate information, it will be displayed here and the **Depth** button in the lower toolbar will be enabled. If the selected file does not have depth calibrate information, it can be created using this function. The user may view, add, and/or change the scale of the x axis between time and depth by selecting the **Time** or **Depth** buttons in the lower toolbar and changing the units using the option menus in the lower toolbar.

Additional “layers” (span of time/depth with one sputtering rate) can also be defined, revised, and deleted. Define (Add) a layer by clicking in the text field labeled Layer and enter a layer name. When the name has been entered, press Enter. The rate field will be displayed (in nanometers per minute) automatically, and the **Add** or **Delete** button will become enabled. Pressing the Add button places an interface “cursor” on the data in the Profile window. This cursor can be dragged, using the left mouse button, to reposition it, if desired. The Depth Calibrate dialog box is updated accordingly.

The File menu in the dialog box has three menu items: Load, Save, and Save As.... Load and Save As both bring up the file selection dialog box for selection of a directory path and filename. Load is used to open another file. Save As is used to save the data file with the new calibration information to a file under a new name. Save is used to save the data file with the new calibration information in the same file. The **WrtFile** button in the lower toolbar updates the original data file with depth calibration information.

Pressing **Cancel** terminates the function without taking any action. Pressing **Exit** closes the dialog box and toolbar and saves the depth calibration information in the dialog box until that data file is closed or MultiPak is exited.

## **Dern**

*See Smooth/Derivative Setup....*

## **Derivative**

*See Smooth/Derivative Setup....*

## **Differentiate**

*See Smooth/Derivative Setup....*

## **Edge Tool**

This function operates only on spectrum data files (.SPE) in the Spectrum windows. When activated from the Tools menu of the Spectrum window, it displays the lower toolbar plus five cursors (two horizontal cursors, two vertical cursors and background cursor). The operator drags the cursors to measure the edge resolution and the peak distance by selecting mode in the **Mode** combo-box.

- **Center** : To display the central coordinate of rectangle surrounded by two horizontal cursors and two vertical cursors at the lower toolbar.
- **Left , Right** : To display the cross coordinate at the lower toolbar between the background cursor and the diagonal line of the rectangle surrounded by two horizontal cursors and two vertical cursors.
- **Between** : To display the distance at the lower toolbar between two vertical cursors.

Click on Paste to paste the coordinate at the lower toolbar on the graph. Pressing Exit closes the Edge Tool.

## **Edit**

The Edit menu contains the Copy To Clipboard function plus other clipboard related functions. For descriptions of the Edit functions, look them up alphabetically in this section of the manual.

## **Element**

*See Region; Subregion; Periodic Table.*

## **Element Label**

*See Labels Option Menu.*

## Energy

Energy, on the right side of the lower toolbar of the Spectrum window, displays the x-axis value of the location of the mouse pointer in the selected spectrum when the window is active. (The window is made active by clicking with the left mouse button on the file name above the data.) The displayed energy value is updated continuously as the mouse pointer is dragged across the spectrum.

*See also* Depth; Time; Intensity.

## Energy Cursor

The Energy Cursor function is controlled by selecting File–Options–Energy Cursor–Select Elements (or –Energy Only, –All Elements, or –Fingerprint). Figure 3-9 shows an example of the energy cursor. Mouse functions for the Energy Cursor function are summarized in Table 3-5.

*Table 3-5. Mouse Functions with Energy Cursor.*

To:	Point At:	Press:
Display elemental transition(s) or energy only	a place within the axes of the data in the Spectrum window	[Shift]-Left
Display elemental transition(s) or energy only and annotate the data when the mouse is released	a place within the axes of the data in the Spectrum window	Right

Clicking [Shift]-left mouse button inside the axes in the Spectrum window displays the Energy Cursor. Dragging the mouse displays transitions (from the Energy Cursor database) located at that energy. When the mouse button is released, no annotation is added.

When the right button is used, the transitions at each energy are also displayed, but when the mouse button is released, the transitions are added to the spectrum display as annotation.

The information displayed is dependent upon the Energy Cursor settings. Three options are available: Energy Only, Select Elements, and All Elements. In the Energy Only mode the binding energy position of the cursor location is displayed. In the All Elements mode all element transitions in the data base at the current energy will be displayed. In the Select Elements mode only the element transition with the largest potential peak will be displayed.<sup>5</sup>

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<sup>5</sup> The Energy Cursor database is not the same as the XPS and AES transition databases listed in the appendices.

### **3: MultiPak Functions**

Selecting File–Options–Energy Cursor–Fingerprint (AES data only) displays a group of vertical lines over the spectrum that represent the relative intensities and positions of the major peaks of a selected element. The “selected” element is that which has a peak<sup>6</sup> similar in location and intensity to the “diagnostic” (currently displayed) peak. This data comes from the *Handbook of Auger Electron Spectroscopy*.<sup>7</sup> This provides quick and visual access to the handbook data stored in MultiPak without having to refer to reference material elsewhere.

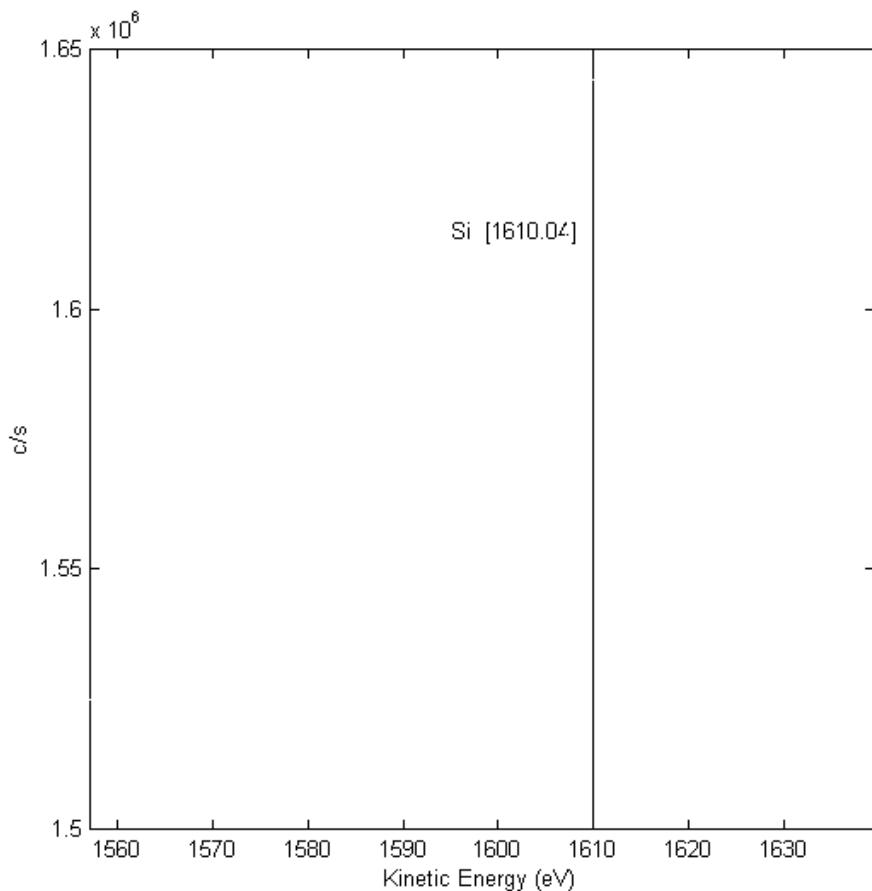
*NOTE: Information supplied by the Fingerprint utility is valid only when working with differentiated AES data.*

The diagnostic peak, typically the most intense peak of an element, is used to determine the initial size of the fingerprint lines. This diagnostic peak line is sized relative to the intensity of the Auger spectrum. The fingerprint lines can be resized (left mouse button) or resized and/or moved using the right mouse button. The sizing capability is designed to be used with overlapping peaks, and the moving capability is designed for peak shifting associated with charging.

Selecting a different element removes any previous fingerprint lines and displays the new fingerprint on the current axis.

The fingerprint display is also available by clicking the right mouse button on an element in the Periodic Table window. Clicking the right mouse button again on the same button removes the fingerprint display.

- 
- 6 Any peak that has the “selected” check box on in its Transition dialog box is considered a “reference” peak; that is, the peak is a candidate in the Fingerprint function.
  - 7 K.D. Childs et al., *Handbook of Auger Electron Spectroscopy*, Third Edition, Physical Electronics: Eden Prairie, 1995.



*Figure 3-9. Example of an Energy Cursor at 1610.04 eV.*

## **Energy Only**

*See Energy Cursor.*

## **ESCA**

MultiPak is always in either ESCA or AES mode, indicating which type of data is currently being reduced. The File–Options menu of each main window allows switching between these two modes. All open files are automatically closed when the ESCA/AES mode is switched in this manner.

MultiPak Version 9 will automatically switch to the correct mode when a file is loaded.

ESCA stands for Electron Spectroscopy for Chemical Analysis, also known as X-ray Photoelectron Spectroscopy (XPS). AES stands for Auger Electron Spectroscopy, sometimes called Scanning Auger Microscopy (SAM).

## Exit MultiPak

Exit MultiPak, available on the File menu, closes all MultiPak files and windows and exits MultiPak.

*See also* Close; Close All; Close and ReOpen.

## Expand

*See* Subregion. *See also* Full Scale.

## Export To

Selecting the Export To function from the File menu of any MultiPak window displays a cascading menu of available formats for file conversion. The available file formats include *PDF...*, *ASCII...*, *ISO...*, *PCX...*, *Color PostScript...*, *B+W PostScript...*, *HPGL...*, *TIFF* (*current image*, *current image + annotation*, *entire window*) and *JPEG* (*current image*, *current image + annotation*, *entire window*). A Save As dialog box opens when a file format is selected. Note: the list of available file formats is different for the Spectrum, Profile, and Map windows.

The user specifies a file name, selects the path for the new file, and presses **OK** when ready (or **Cancel** to escape the function with no action). The Export To command will save a copy of the current file in the selected format. (*See also* Save Current File/Spectrum/Image As....)

A file saved in ASCII CSV (Comma Separated Value) format contains a series of values one per line. The end of a line is the carriage return character. As viewed in Microsoft Excel, the spectral regions appear in adjacent columns each ending with an empty cell. In the CSV file, each data value (cell) is separated by a comma and each line (row) by a carriage return with an empty cell at the end of each column. Cycles or spectra appear in the order in which they were acquired (or in the order in which the spectra were added using the Overlay function in MultiPak, then exported to ASCII format using MultiPak).

The contents of an ASCII file differs for spectrum, map, and profile data, as follows:

- ***Spectrum:***

Cycles or spectra are listed in the block as follows;

- For Spectra in .SPE/.MAP file

- Area name (line 1),
- Area description (line 2),
- Region name (line 3),
- Cycle or spectrum number (line 4),
- Energy and Y value of first data point separated by a comma (lines 5),

### 3: MultiPak Functions

- Remaining Energies and Y values separated by commas, one per line (lines 6 through n),
- Extra carriage return (line n + 1)

Area4	(Area name)
PET	(Area description)
C1s	(Region name)
1	(Cycle or spectrum number)
298.0000,324.2826	(Energy and Data)
297.9500,352.4358	.
297.9000,342.0087	.
297.8500,342.0087	.
297.8000,326.3680	
297.7500,356.6066	
297.7000,344.0941	
297.6500,332.6243	
297.6000,332.6243	
297.5500,329.4962	
297.5000,339.9232	
297.4500,339.9232	

Figure 3-10. Example of Export to ASCII file of spectrum file.

- For Spectra in .PRO/.LIN file
  - Area name (line 1),
  - Area description (line 2),
  - Region name (line 3),
  - Cycle numbers separated comma (line 4),
  - Energy and Y values for each cycle of first data point separated by commas (line 5),
  - Remaining Energies and Y values for each cycle separated by commas, one cycle per line (lines 6 through n),
  - Extra carriage return (line n + 1)

Point1,,,	(Area name)
none,,,	(Area description)
01s,,,	(Region Name)
,1,2,3	(Cycle numbers)
545,48543.332,48846.6641,49389.9961	(Energy and data)
544.8,49086.6641,49466.6641,50093.332	.
544.6,48963.332,48980,49263.332	.
544.4,47866.6641,48876.6641,48890	.
544.2,48233.332,48813.332,49353.332	.
544,49193.332,49469.9961,49256.6641	
543.8,48910,49763.332,49736.6641	
543.6,48450,49053.332,48593.332	
542.4,49626.6641,47760.40220.0061	

Figure 3-11. Example of Export to ASCII file of spectrum in profile data.

When *Row* type is selected in the System Constants dialog box for “ASCII Format”, the blocks are ordered horizontally. If *Column* type is

### 3: MultiPak Functions

selected, the blocks are arranged vertically. The System Constants dialog box is accessed from the following path: File/Options/System Settings.

See “System Settings....”

- **Map:**

- Area name (line 1),
- Area description (line 2),
- Region name (line 3),
- First x value in microns (line 4),
- Step size along x axis (line 5),
- Number of data points (pixels) for on x axis (row) (line 6),
- First y value in microns (line 7),
- Step size along y axis (line 8),
- Number of data points (pixels) for each y value (column) (line 9),
- Y values of all data points on first x axis (row) separated by commas (line 10),
- Y values of all data points on remaining x axis (rows) separated commas, one x axis (row) per line (lines 11 through n),

*NOTE: Annotation on maps is written to the file in the TIFF file format only.*

Area4	(Area name)
Imaged Area	(Area description)
C1s	(Region name)
0.0	(First x value in microns)
5.4	(Step size along x axis)
200	(Number of data points(pixels)for on x axis(row))
0.0	(First y value in microns)
5.4	(Step size along y axis)
151	(Number of data points(pixels) for each y value(column))
6.8900,4.3046,7.3300,5.3600,6.5500,5.9200,6.5717,0.0000,4.5542,9.5692,7.2217,8.9 00,0.0000,5.0500,0.0000,4.6600,4.3800,8.6700,2.0417,6.7492,3.6900,8.1067,1.7600, 5.4600,6.2242,3.776? n 9900 4 1ann & 9902 ? 8900 7 2900,8.3917,6.1700,0.0000,4.5 1300,0.0000,5.4100, ( Map data ) ,2.6500,2.5600,6.5117,5.899 5.2400,0.0000,7.471.....,17,5.3800,5.8000,3.5700,8.5 1.5900,3.4300,5.1600,7.7346,3.2546,8.7200,0.0000,7.2813,0.0000,0.0000,4.8917,0.0 3.4200,2.4446,5.4562,0.0000,5.1946,8.1246,0.0000,2.6400,6.7717,5.2100,4.5500,8.7 2700,7.5683,5.1300,10.2917,3.5400,5.9400,3.5800,4.4300,1.9842,4.3400,0.0000,7.07 7.4867,9.7146,10.6000,9.5946,0.0000,4.7317,7.3617,0.0000,7.0788,0.0000,8.8800,8. 0.0000,7.0346,5.3200,7.4517,4.3300,2.7100,5.0800,6.0246,3.4100,3.5146,1.8700,8.8	

Figure 3-12. Example of Export to ASCII file of map data.

- **Profile:**

- Area name (line 1),
- Area description (line 2),
- Region name (line 3),

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- Number of data points (line 4),
- X and Y value of first data point separated by a comma (line 5),
- Remaining X and Y values, separated by commas, one per line (lines 6 through n),
- Extra carriage return (line n + 1),
- Repeat for next profile.

Point1	(Area Name)
none	(Area description)
01s	(Region name)
151	(Number of data points)
0.0000,92087.5117	(X and Y values)
60.0000,10905.1539	.
120.0000,3947.4940	.
180.0000,5205.9880	.
240.0000,3415.3368	.
300.0000,28775.6635	.
360.0000,25278.5000	.
420.0000 1600 6650	

Figure 3-13. Example of Export to ASCII file of profile.

## Extract Lines...

The Extract Lines... function on the Tools menu (or XLine from the upper toolbar) of the Map window generates spectral data from a line across an ESCA map. Starting this function displays a lower toolbar and adds a blank display labeled Line Profile to the Map window. Table 3-6 lists mouse functions during the Extract Lines... function.

The operator clicks in the map of the current region to define the location of a line. The line's orientation is determined by which radio button (HorizLine, VertLine, or FreeLine) is on (selected) in the lower toolbar. Figure 3-14 shows the result in the Map window, and Figure 3-15 shows the result in the Profile window when Line/New is pressed in the lower toolbar.\* Selecting Window–Map Window in the upper tool bar returns the Map window to the foreground of the desktop.

When HorizLine or VertLine is selected, click the left mouse button on the map to specify the location of the line. (The line automatically stretches from one side to the other or from top to bottom.) The line can be dragged to another location after it has been created.

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\* For horizontal segments, the line profile is created by summing the columns of intensity values (from left to right) within the subregion. Each column is a point on the line profile. For vertical segments, each row is summed, from left to right.

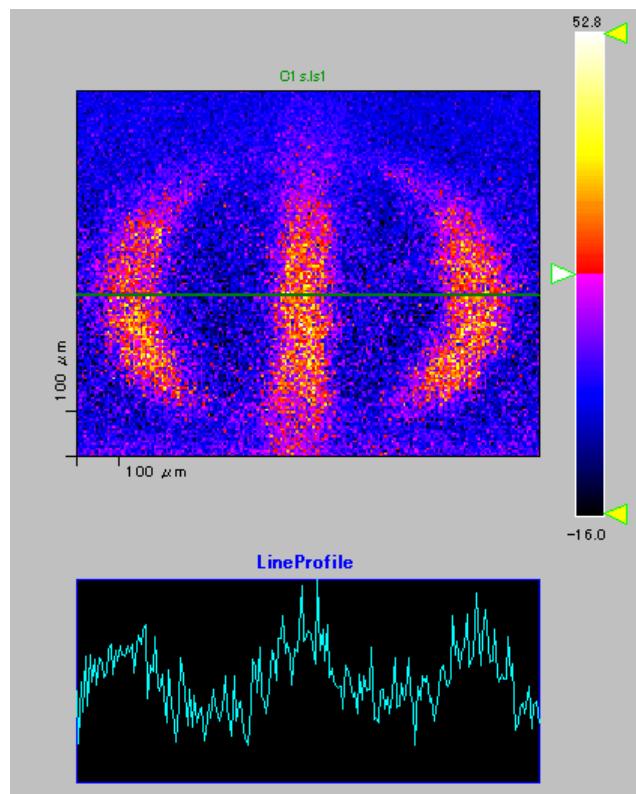
### 3: MultiPak Functions

When FreeLine is selected, click and drag with the left mouse button to define the line. Then, release the mouse button, and click and drag perpendicular to the line to define the width of the area to be summed. The direction in which the mouse is dragged is the direction in which MultiPak will perform the summing to create the line profile.

Pressing **Line/New** creates a line profile in the Profile window and selects it. Pressing **Cut** eliminates the last subregion defined or selected in the Map window. The composite line profile for that subregion is also deleted from the Profile window display.

*Table 3-6. Mouse Functions for the Extract Lines Function.*

To:	Point At:	Press:
Draw lines around a horizontal, vertical, or diagonal rectangular subregion or draw a line	any pixel in the image when HorizLine, VertLine, or FreeLine is selected	Left & drag
Move the subregion	subregion or inside a rectangular subregion	Left & drag
Select the subregion (for moving or cutting)	subregion or inside a subregion	Left
Display the Subregion Properties dialog box	subregion or inside a subregion	[Shift]-Left



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Figure 3-14. Result of Defining a Line with the Extract Lines Function in the Map Window (TONER.MAP).

The **Cancel** button exits the function without taking any action. The **Exit** button terminates the function and leaves the windows in their current state.

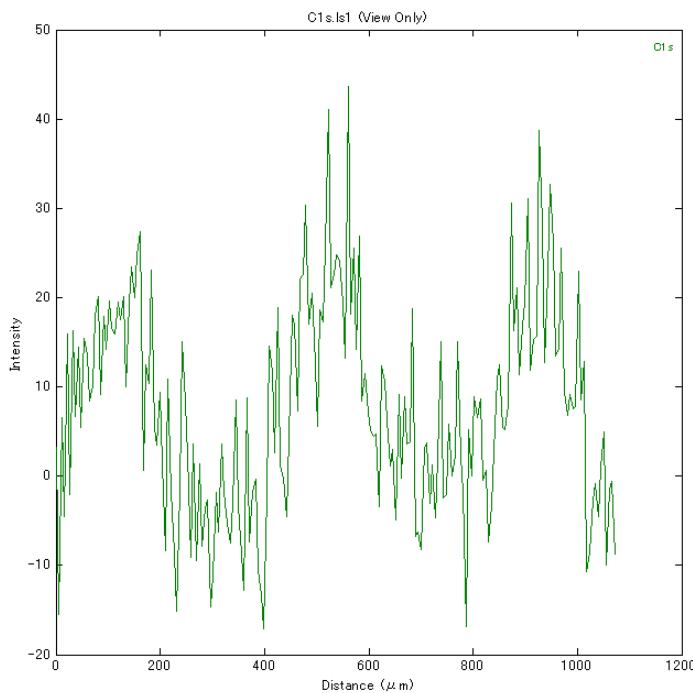


Figure 3-15. Profile Window after Pressing Line/New. (A Binom3 smooth was applied to the line.)

## Extract Spectra...

The Extract Spectra... function is available in both the Map and the Profile window Tools menus and upper toolbars (XSpec). The use of this function for Maps and Profiles is described below.

### Map Window

Selecting Extract Spectra... from the ESCA Map window menu (or XSpec button from the upper toolbar) displays a lower toolbar. Table 3-7 lists mouse functions associated with the Extract Spectra... function in the Map window.

The user selects Polygon or Rectangle and clicks and drags the mouse to define the boundaries of the subregion from which spectra should be extracted. When Rectangle is selected, a subregion can be defined by clicking and holding down the mouse button to establish an anchor point, then dragging the mouse to define the size and shape of the subregion. Release the mouse button when the desired subregion boundaries are displayed.

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When Polygon is selected, a subregion can be defined by clicking, dragging, and releasing the left mouse button to define each side of the polygon. After defining at least two sides of the polygon, close the polygon by clicking once more without moving the mouse.

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Table 3-7. Mouse Functions for Extract Spectra in the Map Window.

To:	Point At:	Press:
Draw lines around a rectangular subregion	any pixel in the image when Rectangle is selected	1. Left & drag to desired size. 2. Press Spec/New.
Draw a polygon around a subregion	any pixel in the image when Polygon is selected	1. Left, drag, and release to draw each side. 2. Left-click to complete the last side. 3. Press Spec/New.
Move the subregion	subregion or inside a rectangular subregion	Left & drag
Select a subregion (for moving or cutting)	subregion or inside a subregion	Left
Display the Subregion Properties dialog box	subregion or inside a subregion	[Shift]-Left

When the **Spec/New** button in the lower toolbar is pressed, new spectra in a new axes are created and selected in the Spectrum window. The new spectra are intensity curves that represent composites of the spectra from all the pixels in the defined subregion. (Each pixel of the map has an energy spectrum stored in its data file.) The spectra can be displayed in either intensity or normalized intensity using the Data–Normalize function in the Spectrum window.

To select a subregion, click on or inside a subregion. Pressing the **Cut** button in the lower toolbar removes the selected subregion (or the last subregion defined) from the Map window. The composite spectrum for that subregion is also deleted from the Spectrum window.

The **Cancel** button exits the function without taking any action. The **Exit** function terminates the function and leaves the windows in their current state.

*See also Spec/New.*

### Profile Window

Selecting the Extract Spectra... function from the Tools menu (or XSpec from the upper toolbar) of the Profile window displays a lower toolbar. Table 3-8 lists mouse functions associated with the Extract Spectra function in the Profile window.

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The user clicks and drags the mouse to create subregions of the profile from which spectra should be extracted. A single profile region can be displayed by clicking on the profile line for that region, or all profiles can be displayed by clicking on the DispAll button in the lower toolbar.

When the **Spec/New** button in the lower toolbar is pressed, a composite spectrum is extracted from each subregion of each visible profile region and displayed in a new axes in the Spectrum window. The spectra can be displayed in either intensity or normalized intensity using the Data-Normalize function in the Spectrum window.

The user can refresh the normalized intensity curve with a different subset of data by manipulating the width and location of the subregion boundaries in the Profile window. In this way, the data may be manipulated until the information of interest has been revealed. New subregions can be defined, added, and manipulated as long as the Extract Spectra toolbar is still displayed in the Profile window.

Composite spectra in the Spectrum window are color coded to match the color of the corresponding subregion boundaries in the Profile window. For example, when only one profile is displayed in the Profile window and only one subregion is defined, only one composite spectrum is displayed in the associated part of the Spectrum window. When one profile in the Profile window is displayed but two subregions have been defined, two color-coded composite spectra will be displayed in the associated part of the Spectrum window. If two profiles in the Profile window are displayed and three subregions are defined, then six composite spectra are displayed in the associated part of the Spectrum window.

*Table 3-8. Mouse Functions for the Extract Spectra Function in the Profile Window.*

To:	Point At:	Press:
Create a subregion	anywhere within the profile axes	Left & drag
Move the boundary of the subregion	subregion boundary	Left & drag
Select the subregion (for moving or cutting)	subregion	Left
Move the subregion	subregion boundary	Right & drag
Toggle the subregion selection	subregion boundary	Right

*NOTE: The colors assigned to each spectrum can be changed in the Data Properties dialog box by clicking on the spectrum using [Shift]-left mouse button.*

To select a subregion, click on a subregion boundary. Pressing the **Cut** button in the lower toolbar eliminates the selected subregion (or the last

subregion defined) in the Profile window. The composite spectrum associated with the subregion is also deleted from the Spectrum window.

The **Cancel** button exits the function without taking any action. The **Exit** function terminates the function and leaves the windows in their current state.

*See also* Spec/New.

## **File**

MultiPak's main File menu contains file management functions like Close, Save As..., Print..., and Options (where the technique is selected plus other functions according to the window from which the menu is opened). For descriptions of these File functions or functions listed on File menus inside dialog boxes or in the Periodic Table, look the functions up alphabetically in Section 3 of this manual.

### **File Comment**

*See Legend.*

### **File Information Setup**

*See Open.*

### **File Name**

*See Legend.*

### **File Types**

*See Open.*

### **Filter...**

The Filter... function, available from the Data menu of the Map window, allows the user to massage or manipulate the selected map in several ways: Smooth, Sharpen, Median, Median+, and Laplacian. Each filter is described briefly below:

- **Smooth**—reduces noise in a map display by replacing each pixel with an equally weighted average of the neighboring pixels, improving the visual presentation and analytical usefulness of the map. (see Appendix A, "Smooth")
- **Sharpen**—subtracts the Laplacian of an image from the image itself. This routine is intended to have a deblurring effect on images. In effect, the routine increases the average steepness of gradients and increases the contrast just at the edges of image features.

- **Median**—assigns a median value (below and above which there are an equal number of values) to each pixel from the values of the surrounding pixels (above, below, to the right of, to the left of, and diagonally adjacent to the pixel). This filter is most useful for the removal of extreme pixel values within an image.
- **Median+**—assigns a median value to each pixel from the values of the pixels above, below, to the right of, and to the left of the pixel. Unlike the Median filter, Median+ does not look at the pixels diagonally adjacent to the pixel.
- **Laplacian**—calculates the linear derivative operator for each pixel and creates from those values a “blurred” (averaged) version of the image.

The option menu ( $3\times 3$ ,  $5\times 5$ ,  $7\times 7$ ) in the lower toolbar determines the level of filtering performed; that is, a representation of the image is arrived at by sampling a matrix of 9 ( $3\times 3$ ) pixels, 25 ( $5\times 5$ ) pixels, or 49 ( $7\times 7$ )pixels. The selected data is actually filtered when the **Filter** button in the lower toolbar is pressed.

*NOTE: Filtering is cumulative; that is, the filter is applied to the currently displayed data, not the original data.*

The filter selected in the lower toolbar becomes the currently available filter in the upper toolbar. For example, the button in the upper toolbar of the Map window will be named “Smo3” with the toolbar set as shown in Figure 3-23. It would be named “Shrp5” if the Sharpen button were turned on and the option menu set to  $5\times 5$ .

Pressing the **Exit** button terminates the function but maintains the last display of the smoothed data. Pressing the **Undo** button restores the display to the display shown the last time the Filter function was exited.

*NOTE: To compare different filter actions, use the Undo function on the Edit menu to restore the original data.*

## Fingerprint

*See Energy Cursor.*

Selecting Fingerprint from the Annotate... lower toolbar, displays the current settings (font, type size, etc.) for Fingerprint annotation, allows the user to change the settings, and applies the displayed settings to the selected annotation (**Apply** button) or all annotation (**Apply All**). Selecting Edit-Clear Annotation–Fingerprint removes any Fingerprint-style annotation from the display.

*See also Annotate....*

## FontSize

*See System Settings.*

## Format...

Refer to “Atomic Concentration Table” earlier in this section for a description of the Format... function on the Atomic Concentration Table submenu.

## Full Scale

The Full Scale functions are available on the View menu of the Spectrum and Profile windows.

If the display of the current data has been changed from its original range (by pressing a region button, for example), selecting the *Full Scale (X and Y)* function will restore the full display of the data. Selecting *Full Scale (Y)* will preserve the x (energy) scale limits and adjust the y display limits so that all data curves are visible.

*NOTE: Full Scale will not return negative values to the display after performing a Data–No Negatives in the Profile window. To restore the negative values use the Close and ReOpen function.*

## FWHM/Area...

The FWHM/Area... function is available from the Tools menu of the Spectrum window. On ESCA files, it computes for the current region the height in counts per second, energy in eV, area in counts per second per eV, FWHM (full width at half maximum) in eV, background noise (signal-to-noise ratio of the background to the right of the peak), and P/N (Peak-To-Noise ratio), as illustrated in Figure 3-16. On AES files, it computes peak-to-peak height in counts per second, energy in eV, and background noise. If the **Calc ISO** box is checked in the lower tool bar, the peak energy measurement will be made using the method described in ISO Standard 15472.

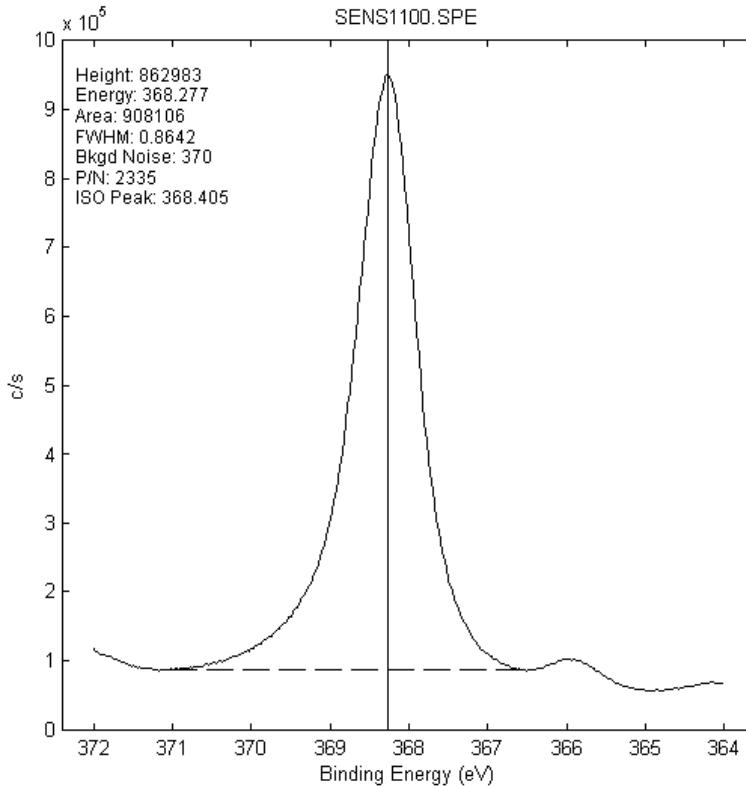
*NOTE: Background noise and P/N (Peak-To-Noise ratio) is calculated as described in Appendix A “FWHM/Area....”*

First, display the desired region by clicking on the region’s button in the lower toolbar of the Spectrum window. Adjust the boundaries of the region and perform any data reduction or manipulation desired. Select FWHM/Area... from the Tools menu. The results are displayed within the axes.

If desired, perform additional data manipulation, and select FWHM/Area... again. The values are updated.

The **Exit** button in the lower toolbar terminates the function. Selecting View–Full Scale (X and Y) restores the window to the original data display.

*See also Print Each Region—FWHM/Area; Appendix A, “FWHM/Area....”*



*Figure 3-16 FWHM/Area... Function Performed on a Carbon Peak in an XPS Spectrum File.*

## **Gray**

*See Color Option Menu.*

## **Green**

*See Annotate...; Color Option Menu; Data Properties.*

## **H He...**

This button is available on the upper toolbar of the Spectrum window. Pressing it restores the display of the periodic table to the foreground of the desktop. An alternative way to bring the Periodic Table to the foreground of the display is to select *Periodic Table* from the *Window* menu on the upper tool bar.

## **Header**

The Header toggle function is available from the View menu of each main window. A check next to this menu item indicates it is on. Turning the header on or off in one window does not affect the header in the other windows.

The header is located in the data display area of the window above the data axes. The information displayed in the first two lines comes from the file of the currently selected data. The third line displays MultiPak information: the name of the current region and the processing history of the region during the current session.

*NOTE: When multiple axes are displayed within the window, only the header associated with the currently selected spectrum is displayed (when Header is on).*

## **Help**

The Help menu contain Mouse Help and About MultiPak. Mouse Help provides a quick glance at how the mouse buttons work in different MultiPak functions. About MultiPak displays the version of the MultiPak software and the copyright information.

## **Hide MultiPak**

Hide MultiPak is available on the Window menu. Use this function to hide all the MultiPak windows in a single action. When Hide MultiPak is selected, the MultiPak *display* closes and a small window-shaped icon labeled “Show MultiPak” is displayed instead.

Clicking on the Show MultiPak icon on the desktop restores the display of the MultiPak windows.

(The Minimize button ( – ) can be used to temporarily iconize an individual window.)

## **Hot Keys**

*See System Settings....*

## **HPGL...**

*See Export To.*

## **Image Enhance...**

The ImageEnhanceSetup... function, is available from the Data menu of the Map Window, This function allows the user to improve the quality of the selected image by adjusting three parameters: Smooth, Sharpen, and

### 3: MultiPak Functions

Background. Selecting the ImageEnhance function from Data menu of the Map Window automatically performs Image enhancement using the parameters specified in the previous Image Enhance Setup....menu.

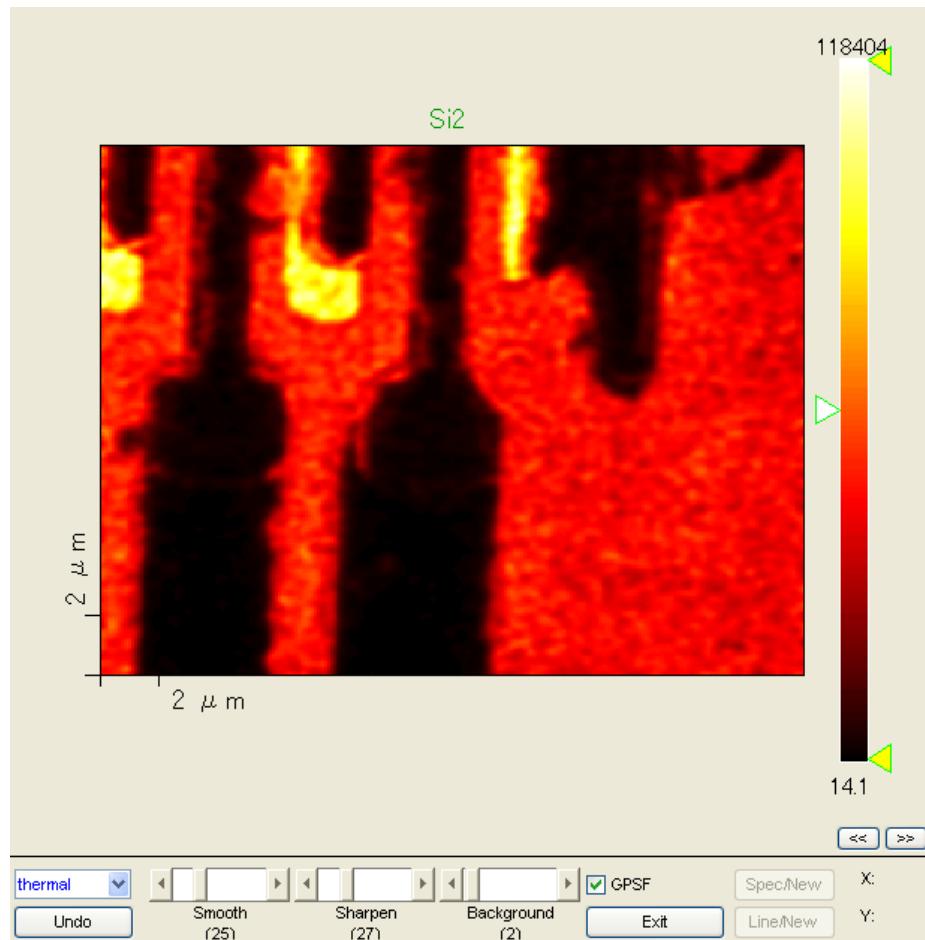


Figure 3-17 ImageEnhance...

- **Smooth** - Reduces noise in an image display by applying a mathematical convolution of the image data
- **Sharpen** - Sharpens edges and improves the display of small features by performing a mathematical deconvolution on the image data
- **Background** - Used to subtract the background from the image
- **GPSF** - If GPSF is selected, the point spread function is made from a Gaussian shape and is suitable for AES. If

GPSF is not selected, the point spread function is made from lorentzian shape and it is suitable for XPS.

The up/down buttons of both sides on the scrollbar provide the ability to quickly make coarse changes. Fine adjustments can be made by clicking and dragging the scroll bar with the mouse. Pressing the Undo button restores the display to the display shown the last time the ImageEnhance function was exited. Pressing the Exit button terminates the function but maintains the image as it was last displayed.

## **Imag/New and Imag/Upd**

Pressing the **Imag/New** button creates a stage map in the Map window from the current data (if the spectral data was acquired from different stage positions) and establishes a direct link between the Spectrum and Map windows. (The **Create/Update Map** button in the Autoreduction Setup dialog box does the same thing.)

*NOTE: A stage map can also be created using the Tools–Stage Map Boundary Setup... function in the Spectrum window.*

Once the link is established or if the spectra are from a MAP file, the button is renamed **Imag/Upd**. The button will be named Imag/Upd until other spectra are selected or another function is activated that breaks the direct link between the data in the Map window and the data in the Spectrum window. Pressing the Imag/Upd button does manually what turning on the Data Link button does automatically: It assures the user that the data displayed in the Map window reflects the current data in the Spectrum window.

*NOTE: .spe files from the Quantum and Quantera currently support the stage mapping capability.*

*See also* Data Link; Stage Map Boundary Setup....

## **Intensity**

Intensity is displayed numerically on the right side of the lower toolbar of the Spectrum and Profile windows when the window is active. The window is made active by clicking with the left mouse button on the file name above the data. The display is continuously updated as the mouse pointer is moved across a selected spectrum. The Intensity field displays the y-axis value in counts per second at the current mouse pointer location.

*See also* Depth; Time.

## Intensity Calibration

Intensity Calibration on the Tools menu of the ESCA Spectrum window has two functions on its cascading menu: *Update File...* and *Calculate....* On the Tools menu of the ESCA Profile window, only *Update File...* is available.

ESCA instrument's transmission function are expressed in two types of model. One is functional model using the transmission function correction coefficients (a and b). The other is interpolated mode. The coefficients are used to generate appropriate sensitivity factors, which are used for atomic concentration calculations (as described in Appendix A, "Sensitivity Factors—Transmission Function Correction.").

Coefficients are calculated from a multiplex data acquisition consists of three energy ranges (two XPS peaks (1000–900 eV, 150–50 eV, 300–500 eV)) using multiple pass energies. In the Spectrum window, MultiPak can compute the coefficients automatically from this data file using the *Calculate...* function. The new coefficients can be written to the data file using the *Calculate* or *Update File* function, if desired, or data reduction can be performed on the file using the new coefficients, as described in the following subsections.

*NOTE: Save the newly calculated transmission function correction coefficients in the acquisition software, so the correct values for the coefficients values are saved with future data files as part of the acquisition process.*

*See also* Appendix A, "Sensitivity Factors—Transmission Function Correction."

### **Calculate...**

The *Calculate...* function is used to view, calculate, and/or change the coefficients. The coefficients are used only on the current file during the current analysis session when *Exit* is pressed in the toolbar, or will be written to the data file permanently when the *Update File...* pushbutton in the dialog box is pressed. Neither action is taken when *Cancel* is pressed in the toolbar.

When the cdata file is opened, *Calculate...* is selected from the Intensity Calibration menu, and the Compute combo box is selected the coefficients are computed automatically. A copper calibration curve, calibration coefficients, and relative standard deviation are displayed, as shown in Figure 3-18. In functional model method the coefficient fields in the toolbar (Coeff. A and Coeff. B) are also updated. Turning off the Compute check box again removes the new curve and data and redisplays the original data file.

### 3: MultiPak Functions

*NOTE: PHI has defined a specific measurement protocol for measuring the transmission function of each instrument type. This protocol defines what data should be collected and how it should be processed using this function.*

Pressing **Cancel** exits the function without updating the data file header or keeping the calculated coefficients in memory. Pressing **Exit** closes the function without updating the current file header, but keeps the coefficients in memory for use on the current file during the current session only (until the file is closed).

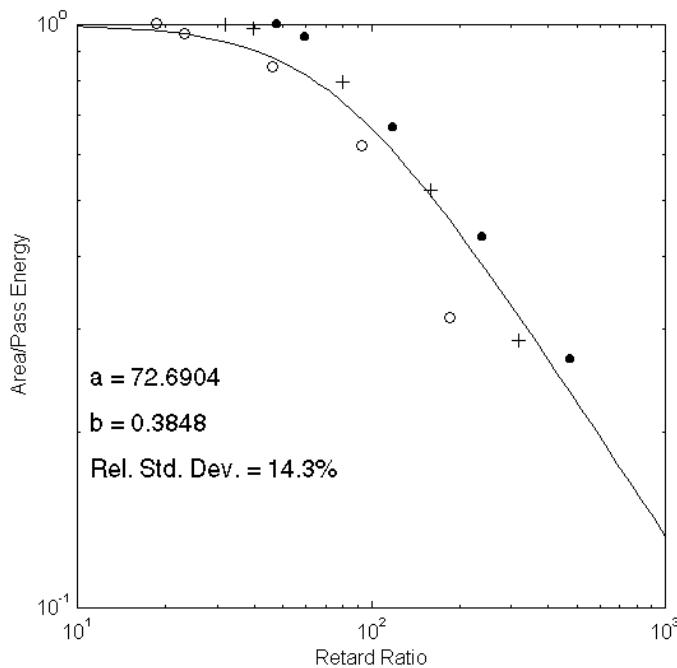


Figure 3-18. Display of Calculated Coefficients a and b.

#### ***Update File...***

Selecting Tools—Intensity Calibration—Update File... displays a dialog box for viewing and/or changing the coefficients (a and b). New coefficients are entered by clicking on the coefficient's text field and typing the new values. The coefficients will be used only on the current file during the current session when **Exit** is pressed in the toolbar, or will be written to the data file permanently when the **Update File** pushbutton in the dialog box is pressed. Neither action is taken when **Cancel** is pressed.

## Intensity Type

The spectral intensity mode is established in the Transition dialog box and can be changed there or in the Analysis Region Properties dialog box. The following intensity types are available:

### **3: MultiPak Functions**

- *Peak Area*—defines a background between the two analysis region boundaries, then calculates the area under the curve and above the background.
- *Peak Height*—defines a background between the two analysis region boundaries, then calculates the y-axis measure from the highest point on the curve to the background.
- *Peak To Peak* (AES only)—calculates the difference between the lowest y point on the curve and the highest y point on the curve.
- *COG*, or center of gravity (ESCA map data in the Spectrum window only)—calculates the centroid of the peak at each pixel and converts the brightness scale to a binding energy scale with high binding energy centroids being brighter.
- *Charge* (ESCA map data in the Spectrum window only)—displays (BE  $\times$  Count Rate) divided by the sum of all pixels.

*See also* Analysis Region Properties; Transition Dialog Box.

## **Iterative Shirley**

The Iterative Shirley background is computed by performing the Shirley background routine five successive times. Each iteration uses the previous iterations background as its background. The background type (Linear, Shirley, Iterative Shirley, or none) is specified in the Analysis Region Properties or Transition dialog box.

*See Appendix A, “Background.”*

*See also* Analysis Region Properties; Transition Dialog Box.

## **Intro Photo Tool...**

The Intro Photo Tool... function, is available from the Data menu of the Map Window. This function is available photo image file only. This function allows the user to zoom out/in , move and measurement. And user can adjust the contrast, threshold and gamma on the image using the color bar on right side.

- **Zoom** - Zoom out/in in image using slide bar. Zoom in operation can also be handled with mouse.
- **Move&Zoom / Measurement** - Select the mouse operation mode. “Move&Zoom” allows user to zoom in or move the image with mouse. “Measurement” allows user to measure the distance between mouse dragging

*start position and end position and paste the measured values annotation on the graph. This annotation will be deleted when updated the image.*

- **Reset-** Pressing the Reset button, back to the image without zoom out / in effects.

Press the Exit button to terminate the function with keeping the last image as it was last displayed.

## **ISO14976 Data Transfer Format**

A standard format for surface analysis data has been specified by the ISO (International Standards Organization) under ISO14976. Use of this format allows data from conforming instruments to be analyzed by any data reduction software that also conforms. It should be noted that programs that convert native data formats to ISO14976 may require the analyst to provide certain fields which are not stored in the data file; the accuracy of information provided for those fields will determine the success or failure of subsequent data analysis.

PHI MultiPak has both import and export functions for the data in the ISO format. MultiPak can read and write the following types of data according to the following procedures. The supported data types for ISO import and export are listed below. Note that all data types allow multiple spectral regions in the same file; however, the maximum number of spectral regions that can be imported or exported with any data file is 20. Unless otherwise noted, data from a single sample position (point) can be read or written to an ISO14976 data file.

### ***Data Import from ISO14976***

- XPS energy spectrum
- AES point, area, or linescan direct energy spectrum
- XPS depth profile energy spectra from multiple data cycles
- AES depth profile direct energy spectra from multiple data cycles

### ***Export to ISO14976***

- XPS energy spectrum
- AES point, area, or linescan direct energy spectrum

### **3: MultiPak Functions**

- XPS depth profile
- AES depth profile direct energy spectra

#### **Procedure**

The File/Import ISO function is available in the Spectrum Window pulldown menus. Select the data file from the dialog box and push [OK] to display the spectrum...

See File/Export To ... ISO to convert the MultiPak data to the ISO14976 format.

## **Labels Option Menu**

The option menu (All Transitions, Element Label, Transition Label, No Labels) displayed at the bottom of the Periodic Table window determines what labels are added to the current spectrum in the Spectrum window when peaks are identified. (The options can be selected only when View–Analysis Region is selected from the upper tool bar of the Periodic Table window.) The results of the selections are the following:

- *All Transitions*—The transition label (e.g., Si2p) for every transition in the database for that element is added at its corresponding energy.
- *Element Label*—The element symbol (e.g., Si for silicon) is added at the energy of the element's most intense transition(s). (These are transitions in the database that have the Peak Label check box checked in the Transition Dialog Box).
- *Transition Label*—The transition label (e.g., Si2p) is added at the energy of the element's most intense transition(s). (These are the transitions in the database that have the Peak Label check box checked in the Transition Dialog Box).
- *No Labels*—No labels are added.

*See also* Transition Dialog Box; Appendices B and C.

## **Landscape**

The View menu in the upper tool bar of the Spectrum and Profile windows provide options for displaying multiple data axes in the same window. (Only one option may be selected at a time.) The options are described below.

*NOTE: The selected option (Landscape, Portrait, Square, or Stack) has no effect on the window when only one spectrum is displayed. A single spectrum within the window is shown in the Square display format.*

### **3: MultiPak Functions**

The Landscape, Portrait, Square, and Stack functions determine the display arrangement as additional files are added to the window, as follows:

- *Landscape* maintains a horizontal orientation for the axes being displayed. A maximum of 36 axes (6 rows by 6 columns) can be displayed in the Landscape orientation.
- *Portrait* maintains a vertical orientation for the axes being displayed. A maximum of 36 axes (6 rows by 6 columns) can be displayed in the Portrait orientation.
- *Square* maintains the block or square orientation for the axes being displayed. A maximum of 36 axes (6 rows by 6 columns) can be displayed in this orientation.
- *Stack* maintains a single column in the landscape format. A maximum of 6 axes (6 rows by 1 column) can be displayed in this orientation. (This option is not available in the Profile window.)

*NOTE: The active data plot in Landscape, Portrait, Square, or Stack is selected (made current) by clicking inside the desired axes (plot) with the left mouse button. The title of the selected (current) plot is displayed in green.*

*See also* Stack Plot; Tile.

## **Laplacian**

*See Filter....*

## **Lapnxn**

*See Filter....*

## **Legend**

Selecting one of the items from the Tools–Legend submenu in the Spectrum window (*File Name, File Comment, Area Number, Area Comment, Point Number, Cycle Number, Region Number*) creates a color coded legend based on the selected information type in the upper right corner of the axes (plot). The color of the text will match the color of the spectra. If the Line Style item in the Tools–Legend submenu in the Spectrum window is also checked, a line of the appropriate color and style is placed to the left of the text.

The style (font, size, etc.) used for Legend annotation can be changed by starting the Annotate... function and selecting Legend from the annotation type option menu in the lower toolbar. Changes to the Legend style can be applied to the selected Legend annotation (**Apply** button) or to all Legend annotation (**Apply All**). Like the other types of annotation, each legend item can be dragged to another location in the plot, if desired.

Selecting Edit–Clear Annotation–Legend removes any Legend annotation from the display.

*See also* Annotate....

## **Line/New and Line/Upd**

The **Line/New** button extracts a line profile from a map and establishes a direct link between the current data in the Map window and the new line display in the Profile window.

Once the link is established by pressing Line/New, the button is renamed **Line/Upd** (update). The button will be named Line/Upd until a new map is selected or another function is activated that breaks the direct link between the data in the Map window and the data in the Profile window. Pressing the Line/Upd button does manually what turning on the Data Link button does automatically: It assures the user that the data displayed in the Profile window reflects the current data in the Map window.

*See also* Data Link; Extract Lines....

## **Linear**

A straight line is drawn between the selected endpoints to form the background shape. The type of background type (Linear, Shirley, Iterative Shirley, or none) is specified in the Analysis Region Properties or Transition dialog box.

*See Appendix A, “Background.”*

*See also* Analysis Region Properties; Transition Dialog Box.

## **Linear Least Squares Fit...**

The Linear Least Squares Fit... (LLS Fit) function is available from the Tools menu and the upper toolbar (LLS) of the Profile and ESCA Map windows. Its operation is described separately below for the Profile and Map windows.

LLS Fit can be applied to profiles, lines, and maps. It calculates spectral intensities by fitting the data measured during profiles, lines, and ESCA maps with standard basis spectra. The basis spectra are selected from the profile line or map data set.

The LLS Fit routine will normally improve dynamic range (reduce noise), although this depends on the signal-to-noise ratio of the data. LLS Fit also allows the extraction from profiles and maps of specific chemical species by selecting basis spectra that contain peak position shifts or shape changes.

*See also* Appendix A, “Linear Least Squares Fit.”

***Profile Window***

When Linear Least Squares Fit... (or LLS) has been activated from the Profile window, the mouse functions summarized in Table 3-9 become available.

The user selects a profile region for fitting by clicking on the profile line or on its label in the upper right corner of the data area. A single basis spectrum can be selected by clicking at the appropriate point along the time/depth scale, or several spectra may be averaged to create the basis if the pointer is dragged while holding the left mouse button down. And a basis spectrum can be loaded from an external spectrum file.

After moving cursor causes all spectra stored with the current profile region (e.g., Si2p) to be fit with the selected basis spectrum. The resultant profile is displayed against the original profile. If the fit looks reasonable (i.e., no wildly negative values and no gross deviations from the original) at all sputter cycles or points in the profile, a single basis spectrum should be sufficient to fit the data. If, however, there are places where the results are poor, select the next basis spectrum from the poorly fit region. Continue until sufficient basis spectra have been selected to produce a good fit to the original profile.

*Table 3-9. Mouse Functions in the Profile Window for LLS Fit.*

To:	Point At:	Press:
Create a subregion	within the axes	Left & drag
Move a subregion boundary	subregion boundary	Left & drag
Reposition a subregion without changing the distance between its boundaries	subregion boundary	Right & drag
View and/or change intensity calculation method or background calculation method	region boundary in the Spectrum window	[Shift]-Left
View subregion type and the lower and upper x coordinates of the subregion	subregion boundary	[Shift]-Left
Remove external basis spectrum	External basis spectrum file name	Left & Drag to outside of axis.

*NOTE: The positions of the analysis region cursors in the spectrum display determine the portion of each spectrum that is used in the fit procedure.*

### **3: MultiPak Functions**

The **ClearFit** button clears the fits associated with the currently displayed profile region. The **ClearAll** button clears all fits associated with all profiles. **DispAll** displays all profiles. (One profile can be displayed by clicking on the profile or on its label in the upper right corner of the data window.)

The **Basic** button will displays file dialog box, retrieves a target spectrum (external basis spectrum) from a spectrum file specified by the user, displays the file name, and operator use external spectrum as basis spectrum.

The **NLLS** button will generate the final result curve by non-linear least square method. Non-linear least square method will fit with consideration for peak shift.

The **Cut** button will delete the region or subregion just defined. The **Cancel** button exits the function without taking any action. The **Exit** function terminates the function and displays all fits as new profiles in the current axes.

#### **Map Window**

Once the LLS Fit function has been activated from the ESCA Map window, the mouse functions summarized in Table 3-10 become available.

In a manner similar to that described under “Profile Window,” the user selects basis spectra from those stored with the map to represent the data.

Click and drag the mouse using the left button to define a rectangular or polygon area on the map. Polygons of any complexity may be drawn by the user. To create a side, click, drag, and release the left mouse button. To close the polygon, click and release the left mouse button *without* moving the mouse: The software fills in the last side of the polygon, so it is not necessary to join the endpoints manually.

### 3: MultiPak Functions

Table 3-10. Mouse Functions in the Map Window for LLS Fit.

To:	Point At:	Press:
Create a rectangular subregion	any pixel in the image when Rectangle is selected	1. Left & drag to desired size. 2. Press Spec/New.
Create a polygon subregion	any pixel in the image when Polygon is selected	1. Left, drag, and release to draw each side. 2. Left-click without moving the mouse to complete the last side. 3. Press Spec/New.
Select a subregion (for moving or cutting)	subregion or inside a subregion	Left
Move a subregion boundary	subregion or inside a subregion	Left & drag
View subregion type and the lower and upper x coordinates of the subregion	subregion boundary	[Shift]-Left

The spectra associated with the pixels in a defined area are summed to create a basis spectrum. Pressing the **Fit** button creates a new map by fitting all spectra stored with the map to the basis spectra. The residual error is displayed in the main map display. If significant features remain in the error map, define subsequent areas for basis spectrum extraction and fit the multiple bases. The component maps are displayed at the bottom of the window.

*NOTE: For AES spectrum Map, negative intensity of result image is truncated to be zero.*

The **Cut** button will delete the currently selected area. The **Cancel** button exits the function without taking any action. The **Exit** function terminates the function and updates the window with the LLS Fit results.

## LineWidth

See Data Properties.

## **LLS**

*See* Linear Least Squares Fit.

## **Load**

*See* Periodic Table.

## **Magenta**

*See* Annotate...; Data Properties.

## **Markers**

Markers are lines associated with annotation. After starting the Annotate... function (by selecting Tools–Annotate... or pressing **ABC** in the upper toolbar), markers can be created by clicking, dragging, and releasing the left mouse button. Text to be associated with the marker can then be typed. To separate the marker from the text, select the marker and then press the **Ungroup** button in the Annotate lower toolbar.

*See also* Annotate....

## **Map Window**

*See* Section 1.

## **Median**

*See* Filter....

## **Med $n \times n$ and Med+ $n \times n$**

*See* Filter....

## **min**

*See* X-Axis Scale.

## **μm**

*See* X-Axis Scale.

## **Monochromator Correction**

The monochromator correction routine is used to minimize the monochromator intensity signature that is visible in XPS maps of a large area. This function is located in the Data menu of the ESCA Map window.

## Montage Viewer...

The Montage Viewer... function, available from the Tools menu of the Spectrum window, it takes all currently displayed spectra and places each region into its own axis. Exiting the Montage Viewer restores the display to its original state. Figures 3-19 and 3-20 show the Spectrum window display before and after Montage Viewer was executed in the Montage Mode for a depth profile file.

The fields of the Montage Viewer dialog box are the following:

- *Current Region*—option menu for selecting the element region that is currently active.
- *Mode*—option menu for selecting tile (two dimensional) or montage (three dimensional) display.
- *Cycle Selection*—type-in boxes for selecting cycles of data: Start, Incr(ement), and End.
- *Energy Range Selection*—type-in boxes for selecting Min or Max of energy range:
- *Perspective*—azimuthal and polar type-in menus to specify the angles used in the Montage display and arrow buttons to change the angle values.
- *Display*—frame (adds opposing axes so the entire plot has a frame around it) or reverse (reverses the order in which the data cycles are displayed) or profile label (display the profile label).
- *Font Size*—option menu to select font size of axes label and element title.
- *Line Width*—option menu to select line thickness of axis frame.
- *DrawingType*—Render Mode: option menu to choice the render mode type of graph. The render mode type will be changed if the rendering of graph is rarely incomplete.
-

### 3: MultiPak Functions

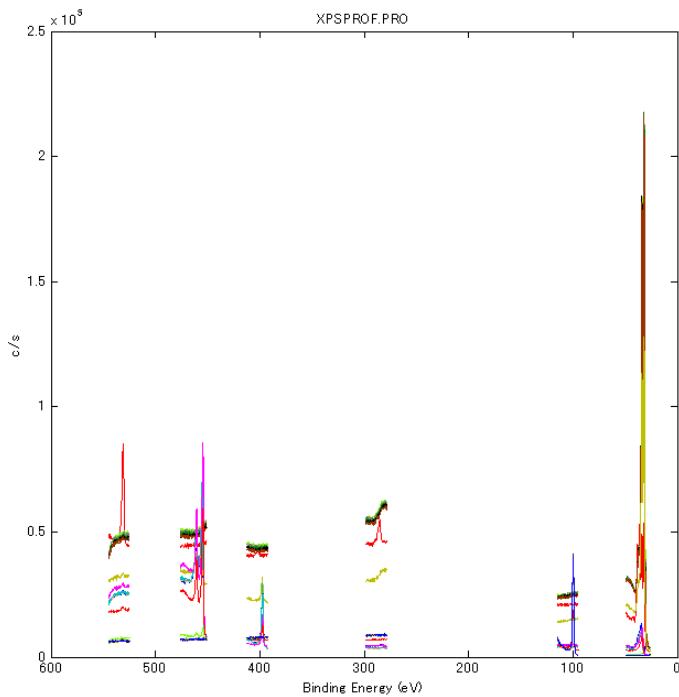


Figure 3-19. Spectrum Window before opening the Montage Viewer.

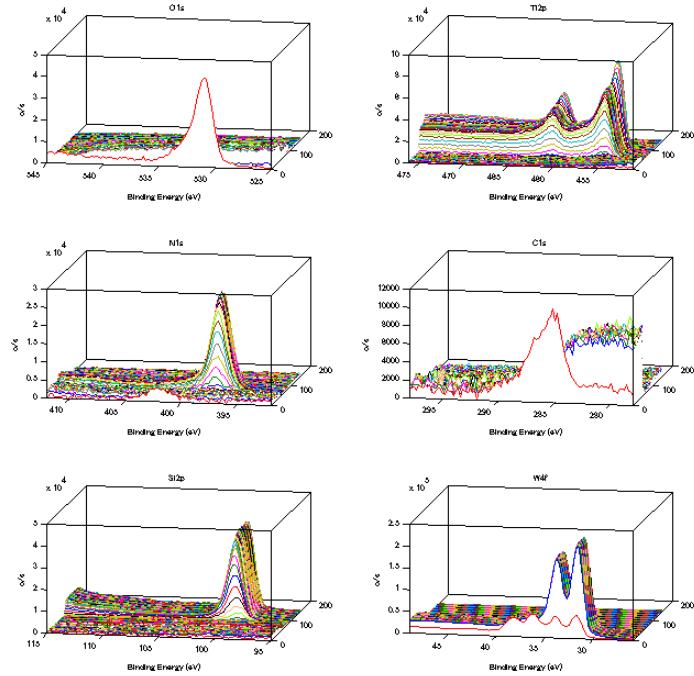


Figure 3-20 Spectrum Window after opening the Montage Viewer and selecting the Montage display Mode.

Pressing the **Apply All** button applies the Montage Viewer parameters set in this dialog box to all data in the window, not just the data currently selected

### **3: MultiPak Functions**

or displayed; **Apply Vis** applies the Montage Viewer parameters set in this dialog box to only the data currently visible in the active window.

Annotation can be added by clicking and typing anywhere within the plot (without having to start the Annotate function).

The Landscape option menu in the lower toolbar determines the layout of multiple axes during the function.

Pressing a region button in the lower toolbar of the Spectrum window will hide or display that region.

Pressing **Exit** closes the lower toolbar.

## **Mouse Help**

Selecting Help–Mouse help displays a list of mouse functions. For complete lists of mouse functions, refer to the discussion of a specific function in Section 3.

*See also* Section 1.

## **Multiple File Open**

*See* Open.

## **New**

*See* Open.

## **New/Ovr**

*See* Open.

## **nm**

*See* X-Axis Scale.

## **No Negatives**

This function is available from the Data menu of the Profile window.

The No Negatives function changes all negative values to zeros. Negative values cannot be restored to the display except by using the Close and ReOpen function to reload the original data file.

## **No Labels**

*See* Labels Option Menu.

## None

The None button in the region bar of the Profile and Map windows turns off all the region buttons.

## Normalize (0 to 1)

The Normalize (0 to 1) function, available from the Tools menu of the Spectrum and Profile windows, toggles between on and off. It is on when a check appears next to it on the menu.

When Normalize is on, all data displayed is scaled to be between 0 and 1. (The highest value is set to one, and the lowest value is set to 0.) When it is not on, data is scaled in counts per second.

## Open

The functions in the File–Open dialog box are described in Table 3-11. When a file is opened, all open MultiPak windows will be refreshed with a display of the new file. The form of the display update depends on the Overlay and View options selected. This dialog box allows selection of more than one file at a time.

Refer to Section 1, “MultiPak Windows,” for a description of file types (and their extensions) that can be opened in each MultiPak window.

*See also* Landscape; Tile.

Table 3-11. *Mouse Functions in the Open Dialog Box.*

To:	Point At:	Press:
Select a file (and deselect any previously selected file(s))	file name	Left
Open a file	file name	Double left
Toggle the selection of the file under the mouse pointer (and leave the other files in their selected state)	file name	Right
Select all files between the highlighted file (even if it has scrolled off the display) and the file under the mouse pointer	file name	[Shift]-left
Select whether the data in the files opened replace, overlay, or are put next to data already displayed in the window	one of the radio buttons along the bottom of the dialog box	Left

### **Autoreduction On Open**

When the Autoreduction On Open check box in the Open dialog box is turned on, the functions selected in the current autoreduction setup dialog box for that file type are performed automatically when a file is opened. (See Autoreduction Setup.)

*NOTE: The processing performed on a file is listed in the third line of the file header.*

### **Data Display Options**

The radio buttons in the Open dialog box affect the display of new data in the Spectrum and Profile windows:

- *New*—Keeps the current data file open and *adds* new data to the Window menu in a separate tile. The data just added to the window becomes the current (selected) spectrum. When Tile is checked (on) in the upper toolbar, all opened data is displayed according to the arrangement checked in the Window menu (Landscape, etc.). When Tile is not checked (off), only the current data is visible.
- *Replace*—Closes the file associated with the current data and *replaces* it with data from the new file.
- *New/Ovr*—Creates a new axes (plot), placing all data together (overlaying data) in this axes. The x and y axes are automatically rescaled to allow the full range and intensity of all data to fill the window. (The Tile setting in the Window menu has no effect when New/Ovr is selected.)
- *Overlay*—adds the new data over (*overlays*) the existing data in the current plot. The y axis is rescaled to show all the y data. (The Tile setting in the Window menu has no effect when Overlay is selected.)

### **File Information Setup Dialog Box**

Pressing the Setup pushbutton in the Open dialog box opens the File Information Setup dialog box, where the user selects or deselects (checks or unchecks) which details about files are listed in the Open dialog box. Pressing **OK** accepts the new selections and closes the dialog box, **Cancel** ignores any changes, and **Apply** displays the changes without saving the changes and closes the dialog box.

## Open Last Acquisition

Selecting Open Last Acquisition from the File menu (or **Acq** from the upper toolbar) automatically finds and opens the data acquisition file most recently created by PHI SmartSoft, PHI *COMPASS*, or PHI PC-ACCESS (if there is one). When regions are defined for the acquisition, those region buttons are displayed in the region toolbar and those elements are turned on automatically in the Periodic Table.

## Options

The File–Options cascading menu contains the selection of techniques (*ESCA* or *AES*) plus the *System Settings...*, *Energy Cursor*, and *Spectrum Skip* functions (depending on the window from which the menu is opened). For descriptions of the Options functions, look them up alphabetically in this section.

## Overlay

*See Open.*

## %

*See page 3-1.*

## %ABC

*See page 3-1.*

## Page

*See Region Buttons.*

## Pan

The Pan Left and Pan Right functions are available from the View menu of the Spectrum and Profile windows. Pan (short for “panoramic”) allows the user to scroll to the *Left* and *Right* to see portions of a spectrum that are currently hidden from view (due to expansion of a part of the spectrum). Panning can also be activated directly by dragging an energy cursor or analysis region cursor beyond the left or right vertical axis.

When dragging the energy cursor or an analysis region cursor, there are three rates of panning based on the distance from the edge of the axis. Either releasing the mouse button or moving the cursor back into the confines of the vertical axes stops the panning.

Selecting Full Scale (X and Y) from the View menu restores the display of the entire unexpanded spectrum.

*See also Full Scale; Zoom.*

## **PCX...**

*See Export To....*

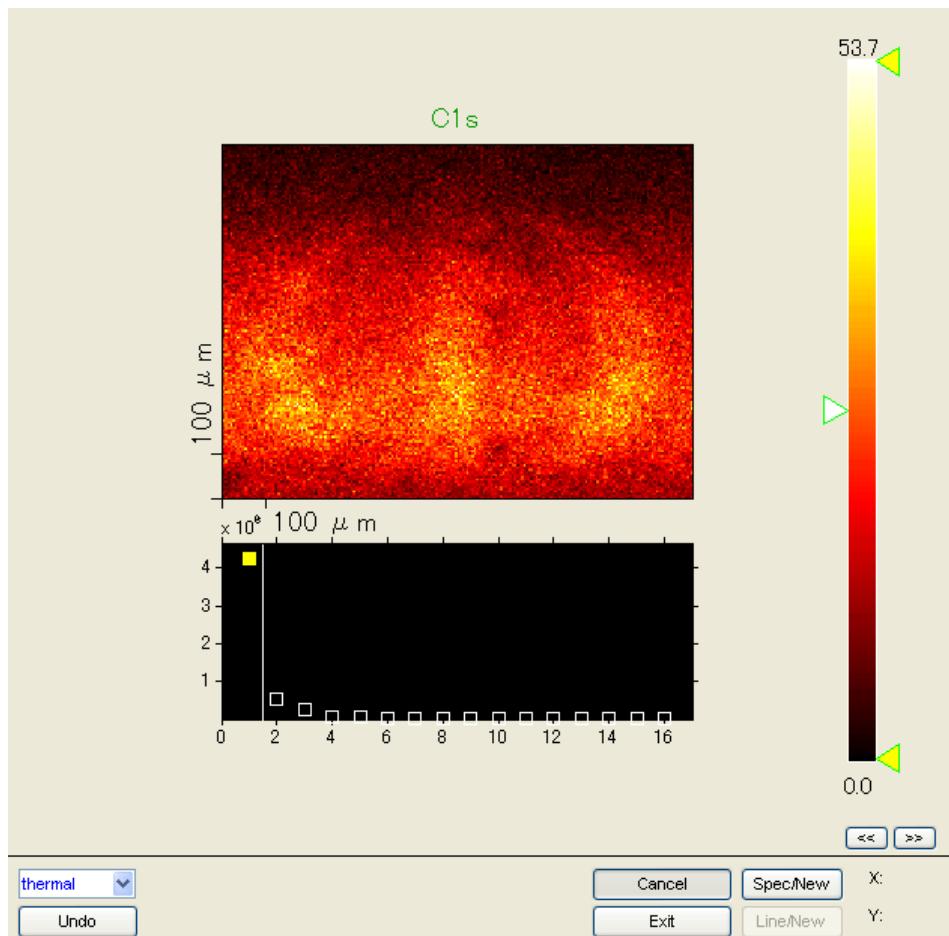
## **PCAImage**

The PCAImage... function, available from the Data menu of the Map Window. This function can only be used with images that contain spectral information at each pixel.

If the quantitative map display mode has been previously selected using the AC% check box on the upper toolbar of the Map Window it will be deactivated upon entering the PCAImage function.

Principal Component Analysis (PCA) is an eigenvector-based multivariate analysis. In this application, PCA is used to evaluate the spectral data stored in each pixel of an XPS map data file and isolate the XPS peak information from the noise information. The output of the routine is a map file that contains spectra with less noise at each pixel. The improved spectral data set is then used to create a map display with improved signal to noise ratio.

When entering this function a map preview is displayed in the middle of the Map Window and the eigenvalue-profile is below the image with a vertical cursor placed between the last principal component identified by the PCA analysis and the first error component. All principal eigenvalue data points are displayed as solid squares, and the error eigenvalue data points are displayed in outlined (open) squares. The PCA-reconstructed image is displayed in the Map window. The user can change the number of principal components by moving the vertical cursor to the left or right. Only the eigenvalues to the left of the cursor will be chosen as principal eigenvalues. The preview image in the Map window is updated automatically as the selection of the number of components changed.

*Figure 3-21 PCA Image...*

Pressing the Spec/New button on the lower toolbar, will display the reconstructed spectrum and error spectrum in the Spectrum Window.

Pressing the Undo button restores the display to its previous condition.

The Cancel button exits this function without taking any action. The Exit button terminates this function, preserves the processed data, and updates the current data display. To restore to the original data file use the Close and Reopen function.

## **Peak**

*See Peak ID; Region; Subregion; Transition Dialog Box.*

## **Peak Area**

*See Intensity Type.*

## Peak Height

*See* Intensity Type.

## Peak

Selecting Peak from the Annotate... lower toolbar displays the current settings (font, type size, etc.) for Peak ID annotation, allows the user to change the settings, and applies the settings to the Peak ID annotation in the selected annotation (**Apply** button) or in all annotation (**Apply All**).

Selecting Edit–Clear Annotation–Peak ID removes any Peak ID-style annotation from the display.

Refer to “Periodic Table” for a description of the Peak ID function on the View menu of the Periodic Table window.

*See also* Annotate...; Peak Identification; Periodic Table.

## Peak Identification/Peak ID

Selecting Peak Identification from the Tools menu or ID from upper toolbar of the Spectrum window automatically matches the peak positions and their relative intensities in the current spectrum with all the peaks and associated intensities stored in MultiPak’s peak identification database for the current technique (ESCA or AES). Peaks that are matched are identified and:

- A button is added to the region bar of the other MultiPak windows for the matching element’s most intense transition,
- A label is added to the spectrum in the Spectrum window according to the selection made in the label options menu at the bottom of the Periodic Table window. (For example, selecting No Labels in the label options menu prevents labels from being added to the spectrum.)

Turning off the Peak Label check box in the Transition dialog box for a specific transition ensures that no label is added for that transition by the Peak ID function. Turning off the Selected check box in the Transition dialog box for a specific transition eliminates that transition from the Peak ID search and prevents a button for that region from appearing in the region bar. All of an element’s transitions can be eliminated from the Peak ID search using the View–Peak ID function in the Periodic Table window. When the Peak ID view of the periodic table is displayed, clicking on an element to change it from green to black eliminates the element from Peak ID searches.

*NOTE: The accuracy of the automated peak identification results may vary depending upon the sample and the analysis conditions. Automated peak identification, which incorporates expert knowledge into a software algorithm, is not a perfect science and continues to evolve. We feel that the current algorithms perform at a level that can benefit our customers even though the identification may not be perfect for all samples. Our goal is to*

### **3: MultiPak Functions**

*provide the best identification routines possible; therefore PHI is committed to the continual improvement of these routines. If you encounter situations where the identification fails, please send PHI Customer Service a copy of the data on a diskette with a description of the failure. PHI will do its best to improve the algorithm in future releases of MultiPak.*

*See also Chemical State ID...; Labels Option Menu; Periodic Table; Transition Dialog Box.*

## **Peak to Peak**

*See Intensity Type.*

## **Periodic Table**

The features of the Periodic Table window are shown in Section 1, “MultiPak Windows,” and are described here.

The **Clear** button at the bottom of the window turns off all the element buttons. The use of the option menu at the bottom of the window is described in “Labels Option Menu.”

*See also Section 1, “MultiPak Windows;” Labels Option Menu; Load; Region; Save; Save As...; Transition Dialog Box.*

### **File Menu**

The window’s File menu has three functions (*Load...*, *Save*, and *Save As...*).

*Load...* allows the user to change current database. Database files originally installed are XPS.EDB and AES.EDB. AES.EDB is the database file of elemental relative sensitivity factors (ERSF). To use the database user edited and save as, select that database file.

*Save* writes all changes made during the current session to the current database, thereby changing the database permanently.

*Save As...* allows the user to save database changes to a new file name, thereby leaving the original or current database intact.

The following database file originally installed in MultiPak, XPS.EDB is assigned the default XPS database and AES.EDB is assigned the default AES database.

*XPS.EDB:* XPS relative sensitivity factor

*AES.EDB:* AES relative sensitivity factor for CMA analyzer.

### **3: MultiPak Functions**

*AES CU.EDB*: AES relative sensitivity factor base on Cu1 in 10kV, they are equivalent to AES.EDB

*AES\_CMASCA.EDB*: AES relative sensitivity factor for both CMA and SCA analyzer.

*AES\_AMRSF.EDB*: AES average matrix relative sensitivity factor for CMA analyzer.

*AES\_CMASCA\_AMRSF.EDB*: AES average matrix relative sensitivity factor for Both CMA and SCA analyzer.

**NOTE:** The values in the originally installed XPS database are listed in Appendix B. That of AES are in Appendix C.

The arithmetic method to convert from CMA's relative sensitivity factor s to SCA's ones is built in MultiPak , hence user can get the atomic quantity of AES data acquired with SCA analyzer under the condition selected AES.EDB database file or AMES\_AMRSF.EDB, on converting CMA's relative sensitivity factors into SCA's ones. In this case, the warning message dialog to be used conversion relative sensitivity factors is displayed. The resultant of atomic concentration is corresponded to that by calculated with AES\_CMASCA.EDB or AES\_CMASCA\_AMRSF.EDB. The discrepancy between with AES.EDB and with AES\_CMASCA.EDB is to enable to edit and check the value of SCA's relative sensitivity factor in the transition dialog box when selected AES\_CMASCA.EDB.

To use an average matrix relative sensitivity factor, it is necessary to select the database right file, AES\_AMRSD.EDB or AES\_CMASCA\_AMRSF.EDB.

#### ***View Menu***

The View menu has three options: *Analysis Region* (default), *Peak ID*, and *Autoreduction*, described below.

*View–Analysis Region* is always selected unless the user selects Peak ID or Autoreduction. The Periodic Table window automatically reverts back to Analysis Region mode when another function is selected in MultiPak.

With Analysis Region selected, clicking on an element in the Periodic Table window adds a button for that element's "Selected" transition(s) to the region bar of the other MultiPak windows.

### **3: MultiPak Functions**

Selecting View–Peak ID from the Periodic Table window allows the user to view and change which elements are excluded from an automatic Peak ID search. Green indicates that the transitions for that element are to be included in the search. Toggling an element button to off (black) excludes those transitions from the automatic Peak ID search. An *automatic* Peak ID search is performed when one of the following actions occurs:

- Tools–Peak Identification is started from the Spectrum window menu,
- Auto Reduction Setup is processed with Peak ID–Automatic turned on in the setup dialog box.

*NOTE: An element's Automatic Peak ID state will remain permanently set until manually changed again using View–Peak ID.*

Selecting View–Autoreduction from the Periodic Table window allows the user to view and change which elements are included in a user-defined Peak ID that is performed as part of an Auto Reduction routine. Green indicates that the transitions for that element are to be available for Peak ID. Toggling an element button to off (black) eliminates those transitions from the user-defined Peak ID. A *user-defined* Peak ID is performed when an Autoreduction Setup is processed with Peak ID–User-Defined turned on in the setup dialog box.

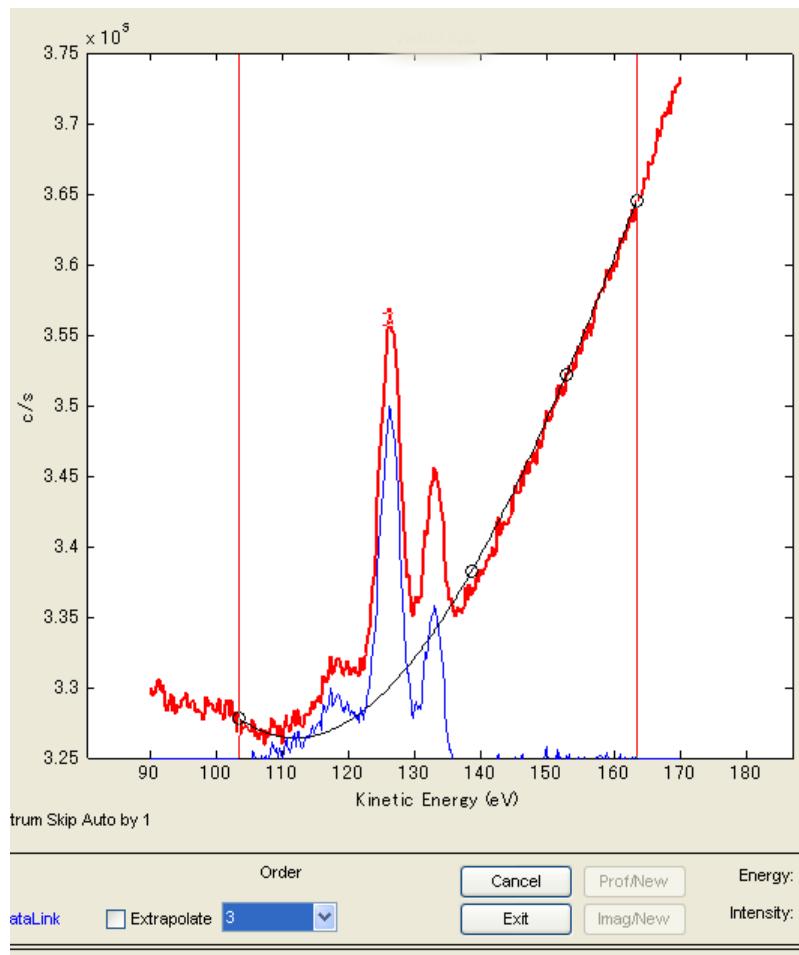
## **Point Number**

*See Legend.*

## **Portrait**

*See Landscape.*

## **Polynomial Background**



*Figure 3-22    Polynomial Background Window*

### **Polynomial Background:**

A polynomial function fitted to points on the energy spectral background. Subtraction of this background from the spectrum then allows an estimate of the area under the peak – note that this does not remove the inelastically-scattered electron background from the peak, however, it gives an estimate of the shape of the broadly scattered primary beam background. The function fitted is given as

$$a_n x^n + a_{n-1} x^{(n-1)} + \dots + a_1 x + c \quad (1)$$

### **Polynomial Order:**

The value of n in the Eq. 1.

### **Extrapolation Mode:**

Allows a reduced order polynomial function to be extrapolated to the low energy side of the current adjuster node. For example, if the analyst has specified order n = 3, then there will be four (4) adjuster nodes numbered 1

– 4, in order, from low to high kinetic energy and, in extrapolation mode, adjusting (e.g.) Node 2 will fit a polynomial of  $n = 2$  using Nodes 2 – 4 and the background to the low energy side of Node 2 is extrapolated from this fit. This feature can be useful if the spectrum range available for fitting to the low energy side of the peak is inadequate.

#### **Adjuster Node:**

The placement of the points on the spectral background to define the polynomial function is currently done manually by the analyst using the “adjuster nodes” (black circles) shown in Figure 3-22. Click & drag a node to position that background-defining point. The background is drawn as the adjuster node is moved and the subtracted spectrum is displayed.

#### **Define the Background**

Select the spectrum to be corrected. Enter the polynomial background fit application, **Data > Polynomial Subtraction**. The display will be as shown in Figure 3-22.

Enter the desired polynomial order in the “Order” entry box. The order can be from 1 (flat line) to 4 (five adjuster nodes will be displayed). Use the minimum order required to fit the background adequately.

Adjust the nodes to achieve the desired background shape against the spectrum; use the background-subtracted spectrum display to determine the best positions.

Press **Exit** to return to the top MultiPak level.

## **Print...**

The Print... function settings, available from the File menu of the main Multipak windows, affects prints made from that MultiPak window only.

This function’s dialog box is used to set the print parameters and to print the current display (to a printer or to a file). The Print dialog box features are the following:

- *Destination*—
  - Printer drop-down menu: Black And White or Color.
  - File drop-down menu: PCX converts and saves the file in a bit-mapped graphics format; ColorPostScript converts and saves the file in color for output to a color printer. B+WPostScript converts and saves the file in black and white format for output to a black and white printer. HPGL converts and saves the file in Hewlett-Packard

Graphics Language for output to a pen plotter compatible with the HPGL graphics format or to another application that accepts HPGL files. TIFF (Map window only) converts and saves the file in the Tagged Image File Format for graphics. (TIFF files are often black and white images.)

After selecting a file type and Save the Print To File dialog box opens. Specify the file name and directory where the file is to be saved.

- *Orientation*—defines the spectrum orientation (portrait or landscape) for printing.
- *Background*—defines the background color (white or Black) for printing.
- *Paper Size*—usletter (8.5×11 in.) or a4letter (9×14 in.).

**Select Printer** allows the user to change the current printer. **OK** saves the settings, does not perform a print, and closes the Print Setup dialog box. **Print** saves the settings of the dialog box and sends the current window to the printer (or writes it to a file). **Cancel** closes the dialog box without saving any changes to the dialog box.

Select ‘Classic’ option in [System Settings...—Print Mode] menu, a print layout is similar as the one of Version 6 in single spectrum printing.

*See also* Export To...; Print in B+W; Print in Color.

## Print Each Axis

This function, available on the Tools menu in the Spectrum window, prints each axis (plot) in the Spectrum window on a separate page.

## Print Each Region, Print Each Region—FWHM/Area

These functions, available on the Tools menu in the Spectrum window, automatically print each region in the file, either in the normal view (Print Each Region) or in the FWHM/Area view (Print Each Region—FWHM/Area). If multiple spectra are present for the same region, all spectra will be printed in the Print Each Region mode and the first spectrum will be printed in the Print Each Region-FWHM/Area mode.

## Print Each Map

This function, available on the Tools menu in the Map window, automatically prints each map, one map per page.

## **Print in B+W**

Selecting File–Print in B+W prints the current display in black and white to the currently defined printer.

## **Print in Color**

Selecting File–Print in Color prints the current display in color to the currently defined printer. (Colors will appear as different shades of gray on a black-and-white printer.)

## **Profile Window**

*See Section 1, “MultiPak Windows.”*

## **Prof/New and Prof/Upd**

Pressing the **Prof/New** button creates a new profile from the current data and establishes a direct link between the current data in the Spectrum window and the display in the Profile window.

Once the link is established by pressing Prof/New, the button is renamed Prof/Upd (update). The button will be named **Prof/Upd** until other spectra are selected or another function is activated that breaks the direct link between the data in the Spectrum window and the data in the Profile window. Pressing the Prof/Upd button does manually what turning on the Data Link button does automatically: It assures the user that the data displayed in the Profile window reflects the current data in the Spectrum window.

*See also Data Link.*

## **Pseudo**

*See Color Option Menu.*

## **Quick Keys**

*See System Settings....*

## **Quick Key Definition...**

*See Atomic Concentration Table.*

## **ReColor**

ReColor is available from the Tools menu of the Spectrum window on the PC.

### **3: MultiPak Functions**

MultiPak assigns one of eleven colors to each individual spectrum in a data display. The colors are assigned in a repeating sequence. Using ReColor allows the user to assign a new color to a selected spectrum.

To do this without using ReColor, the user can select an individual spectrum from a data display using [Shift]-left mouse button to display the Data Properties dialog box. After the user has picked a new color for this particular spectrum and pressed OK in the dialog box, MultiPak refreshes the display with recolored spectra.

## **Red**

*See Annotate...; Color Option Menu; Data Properties.*

## **Region**

The term “region” refers to an analysis region. A region’s definition comes from the data acquisition file and from the MultiPak’s transition database of spectral data. (A transition’s definition can be modified in MultiPak for analysis purposes.) Press on an element in the Periodic Table window to add or eliminate a region to or from the current analysis. Table 3-12 lists operations of the mouse when region boundaries are displayed.

*See also Analysis Region Properties; Region Buttons; Region Cursors; Subregion; Transition Dialog Box.*

*Table 3-12. Mouse Functions for Regions and Region Boundaries.*

To:	Point At:	Press:
Select a region	button in the region bar	Left
Add a region to the region bar	button in the Periodic Table	Left
View region boundaries	View–Region Cursors	Left
Hide region boundaries	View–Region Cursors	Left
Move region boundary	region boundary	Left & drag
Move both region boundaries	region boundary	Right & drag
Restore the full display to the display after viewing a subregion	region button in lower toolbar	Left
View and/or change intensity type or background type	region boundary	[Shift]-Left

## **Region Buttons**

The buttons in the region bar (below the lower toolbar) are called region buttons. They are turned on and off by clicking to zoom into a specific

region. (The full display may be restored by clicking on the region button again or by selecting View-Full Scale.)

When there are more than 12 regions, a Page button for scrolling is displayed in the region toolbar.

*See also* Subregion.

## **Region Cursors**

Region Cursors is available on the View menu of the Spectrum window. When it is on, region boundaries will be displayed. When it is not on, region boundaries will not be displayed.

*NOTE: Region boundaries are also not displayed for transitions whose Selected boxes are turned off. See Transition Dialog Box.*

*See also* Region; Region Buttons; Transition Dialog Box.

## **Region Number**

*See* Legend.

## **Replace**

*See* Open.

## **RGB Overlay**

The RGB Overlay function is used to create an overlay image of red, green and blue images. RGB Overlay is available on the Tools menu of the Map window.

The operator message “No RGB Maps Found” will be shown if maps of at least two of the colors red, green, and blue are not displayed.

The new image will be named with a combination of the names of the red/green/blue images used in the RGB Overlay function. Note that the color bar of the RGB Overlay image has the number 1 at the bottom and number 48 at the top. These are the minimum (1) and maximum (48) intensities that are assigned to image pixels when a single color is assigned to an image.

MultiPak will process the first red/green/blue image it encounters (going in a Landscape order), the second red/green/blue image (not in the same color as the first image), and the third red/green/blue image (if there is one and it is not in the same color as the previous two images). It combines them into a single red and green and blue image.

**S**

*See X-Axis Scale.*

## **Satellite Subtract**

The Satellite Subtract function is intended for use on ESCA data files that were obtained with a non-monochromatic Al or Mg source. The function automatically subtracts x-ray satellites and is available from the Data menu in the ESCA Spectrum window.

*See also Appendix A.*

## **Save**

For descriptions of the Save function on File menus inside dialog boxes or in the Periodic Table, look the functions up alphabetically in Section 3.

*See also Periodic Table; Save As...;*

## **Save As...**

For descriptions of the Save As... function on File menus inside dialog boxes or in the Periodic Table, look the functions up alphabetically in Section 3.

Selecting this function from the File menu of the Periodic Table window allows changes to a database to be saved to a new database with a different name.

*See also Periodic Table.*

## **Save Current File As...**

Selecting Save Current File As... from the File menu of the Spectrum, Profile, or Map window opens the Save Data File dialog box. The operator specifies a file name and directory where the file is to be saved. If the extension is not specified, one is added to the file name automatically. When OK is pressed, all data originally from the file containing the current (selected) data are saved in their current state.

This function makes it possible to maintain a processing history with a data file that includes the following: spectrum shifts, depth calibration information, changes to transmission coefficients, differentiation, changes to analysis region cursor positions, LLS result, TFA result, added regions and image brightness, contrast, and threshold.

*See also Export To.*

## Save Current Spectrum/Image As...

Selecting Save Current Spectrum As... or Save Current Image As... from the File menu of the Spectrum or Map window allows an individual spectrum or map to be saved to a new data file. When the function is selected, the Save Current Data dialog box is displayed. The operator specifies a file name and directory where the spectrum or map is to be saved. When OK is pressed, the current (selected) data are saved to the new file. (If the extension is not specified, one is added to the file name automatically.)

*See also* Export To.

## Scatter Diagram...

Scatter Diagrams, available from the Tools menu of the Map window, provide a method for separating and displaying different chemical phases from two elemental maps acquired over the same area under identical conditions.

A scatter diagram is a two-dimensional (2D) histogram created from two elemental maps that displays the distribution of relative intensities in the two maps. The axes of this 2D histogram are the intensities in the elemental maps, and the value at each pixel is the number of times that corresponding pixels in the two maps have the specified intensities. For example, a scatter diagram that displays a diagonal line of intensity indicates that the two maps have varying intensity within each map but have approximately the same intensity at corresponding pixels. A scatter diagram that displays an anti-diagonal line of intensity indicates that the two maps have complementary intensities at corresponding pixels; that is, when one element shows high intensity, the other element shows low intensity.

A cluster of intensity in a scatter diagram often indicates the presence of a chemical phase containing specific relative amounts of the two elements. A “phase” map can be created from a scatter diagram by displaying a map of the same size as the original elemental maps that shows which pixels have intensities that correspond to a cluster in the scatter diagram. This phase map shows the parts of the original maps that contain a particular phase.

Tables 3-13 and 3-14 summarize some of the mouse functions during the Scatter Diagram function.

*NOTE: The two source images must have the same physical size and location on the sample surface and have same pixel resolution.*

*NOTE: Certain images, such as derived maps (RGB overlay, LLS map, scatter plot, phase maps), cannot be used as source maps for a scatter plot.*

### 3: MultiPak Functions

*Table 3-13. Mouse Functions for the Scatter Diagram... Function in Source Map Mode.*

To:	Point At:	Press:
Select a source map or scatter diagram	map or scatter diagram	Left

*Table 3-14. Mouse Functions for the Scatter Diagram... Function in Phase Map Mode.*

To:	Point At:	Press:
Create a phase map from a rectangular cluster region	scatter diagram	<ol style="list-style-type: none"> <li>1. Left and Drag to define rectangle</li> <li>2. Click on Create button</li> </ol>
Create a phase map from a polygonal cluster region	scatter diagram	<ol style="list-style-type: none"> <li>1. Left and Drag to define each side of polygon</li> <li>2. Click and release without moving mouse to close polygon.</li> <li>3. Click on Create button</li> </ol>
Move a cluster region	inside of cluster region	Left & drag
Select a cluster region (for moving or deleting)	inside of cluster region	Left
Change the phase map color by displaying the Analysis Region Properties dialog box	inside of cluster region	Shift-Left

Selecting Tools–Scatter Diagram... tiles the images (if they are not already tiled) and opens the lower toolbar in Source Map mode.

To create a scatter diagram, first select two source maps by clicking on them with the left mouse button. Then, click on the **Create** button in the lower toolbar. This creates a scatter diagram and selects it. The **FlipXY** button in the lower toolbar can, if desired, be used to exchange the X and Y axes in the scatter diagram.

To create one or more phase maps from a scatter diagram, select the scatter diagram by clicking on it with the left mouse button. Then, enter phase map mode by clicking on the **PhaseMap** button in the lower toolbar. The scatter diagram will be displayed in the map window with one-dimensional

histograms above and to the right and with four phase map preview axes below it.

Next, select Rectangle or Polygon to define the shape of the cluster regions to be defined and create a rectangular or polygonal region around each cluster in the phase map by clicking and dragging the mouse as described in Table 3-19. Press the **Create** button in the lower toolbar to create a phase map for each cluster region and display them in the four preview axes.

If the **Overlay** checkbox in the lower toolbar is checked, an additional phase map will be created that is made by overlaying all the individual phase maps. The << and >> buttons in the lower toolbar can be used to display hidden phase maps if more than four were created. To delete a phase map, select the cluster region of the phase map by clicking on it with the left mouse button, then pressing **Delete** in the lower toolbar.

To create or work with another scatter diagram, select the **SourceMap** button to return to source map mode where new scatter diagrams can be created.

To exit Scatter Diagrams, select either the **Cancel** button in the lower toolbar to discard all work, or the **Exit** button to preserve the scatter diagrams and phase maps that have been created during the application. After exiting, scatter diagrams and phase maps can be tiled, untiled, printed, etc., like any other image in the map window.

## Select Spectra...

Starting the Select Spectra... function, available on the Tools menu of the Spectrum window, opens the lower toolbar and the selection slider is displayed to the right of the data. Figure 3-23 shows the slider and its small horizontal “cursors” in different states. The operator may use the toolbar buttons, selection slider, or both to change how many and which spectra are displayed at one time. Options available for using the selection slider to select a different spectrum or spectra are shown in Figure 3-24.

When ShowAll is selected, all spectra from the current region are displayed, and the selection slider displays two horizontal cursors that can be dragged to change the range of spectra displayed. When ShowOne is selected, only one spectrum is displayed at a time, and the selection slider displays one horizontal cursor that can be dragged to select the desired spectrum.

Noncontiguous spectra may be selected using the Select and Unselect buttons in the lower toolbar. The **Select** button selects all visible spectra, and the **Unselect** button unselects all visible spectra. Selected spectra are displayed in color, and unselected spectra are displayed in gray.

### 3: MultiPak Functions

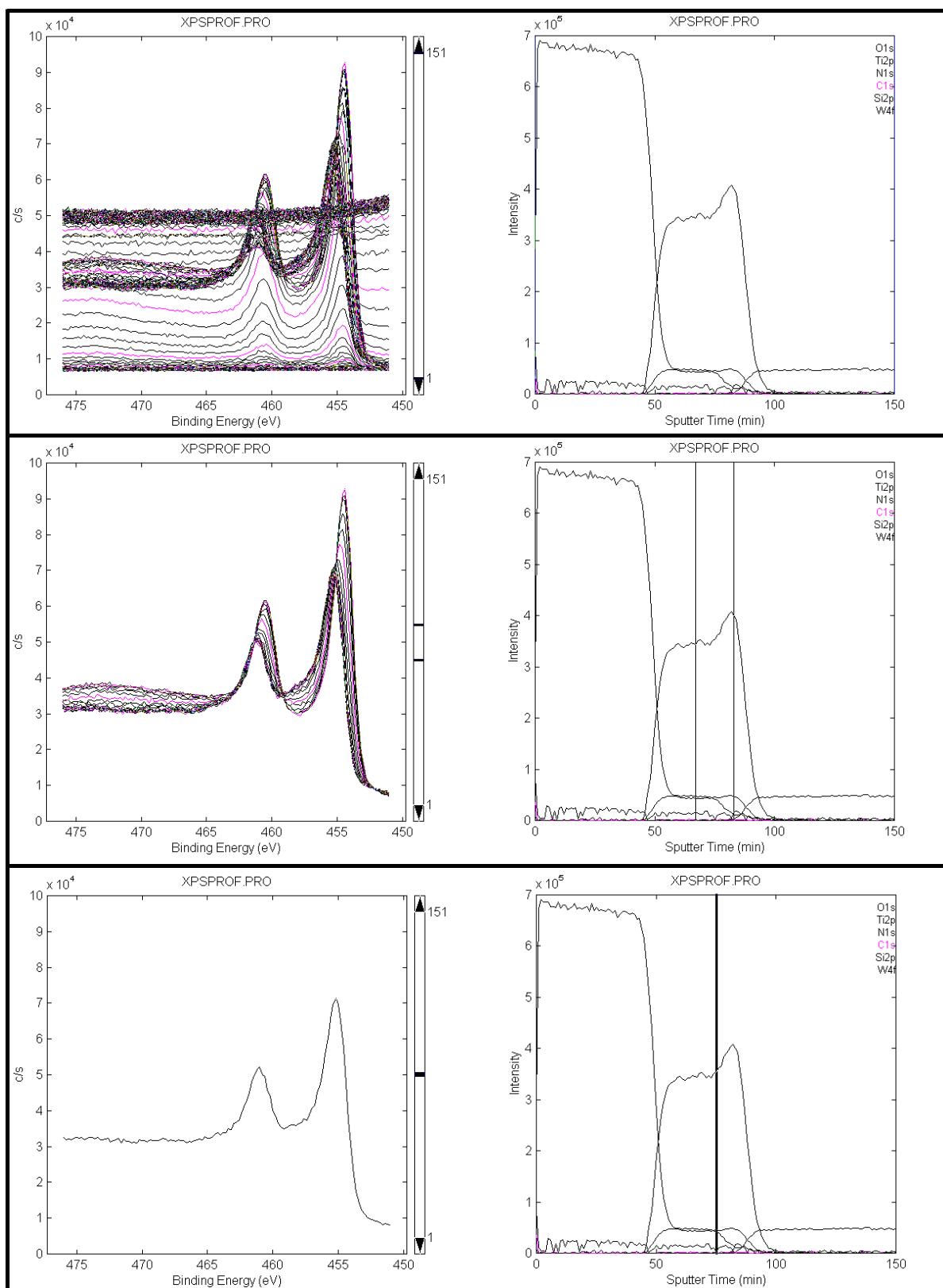
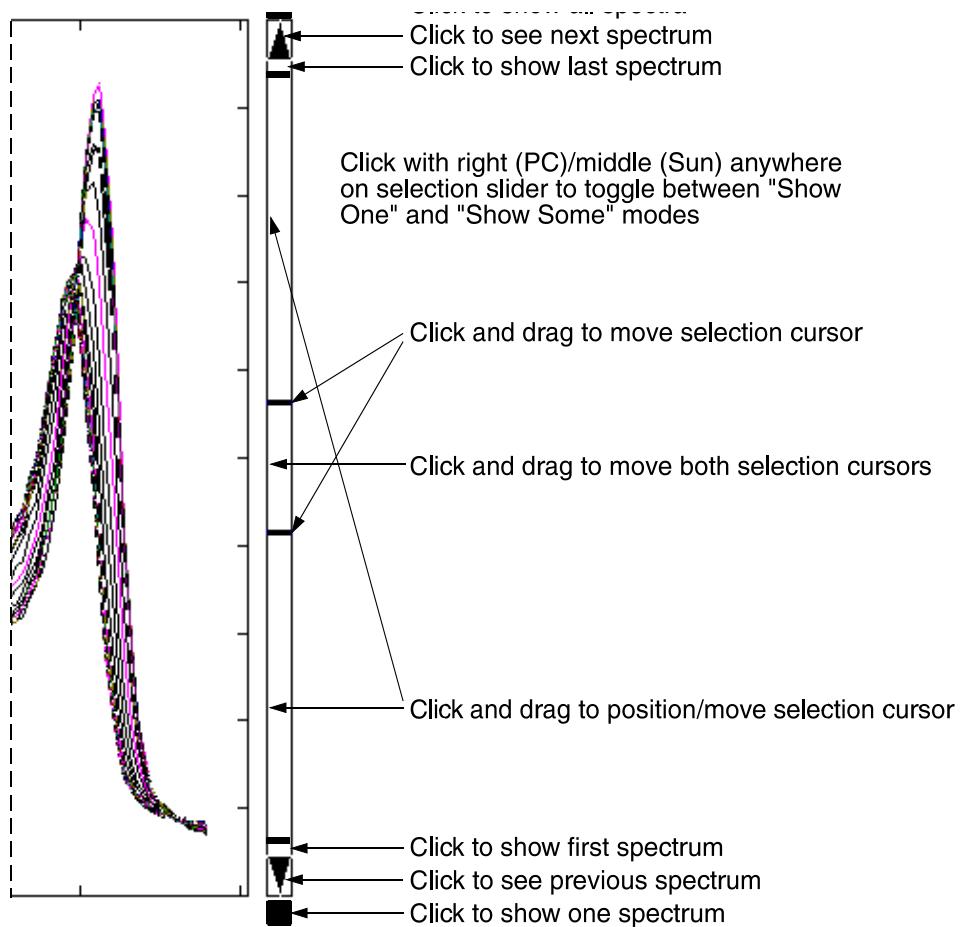


Figure 3-23. Selection Slider in Three States in the Spectrum (left) and Profile (right) Windows:  
ShowAll (top), show some (middle), and ShowOne (bottom).



*Figure 3-24. Options Using the Selection Slider.*

The settings of the Cycle and Area check boxes control what other spectra in other regions are selected at the same time.

Note that, when the current data in the Spectrum window are linked to the Profile window, the data shown in the Profile window are delineated by vertical “cursors” that match the cursors in the Spectrum window’s selection slider. Clicking and dragging the Profile window’s vertical cursor(s) also moves the corresponding horizontal cursor(s) in the Spectrum window.

*See also* Data Link; Extract; Prof/New; Spec/New; Shift.

## Selected Elements

*See* Energy Cursor.

## Selection Slider

Selecting this function from the View menu of the Spectrum window turns the selection slider on and off.

*See Select Spectra....*

## **SGn**

*See Smooth/Derivative Setup....*

## **Sharpen**

*See Filter....*

## **Shift**

The Shift function from the Data menu of the Spectrum window automatically shifts the data in all regions based on the data in the selected region: MultiPak finds the energy of the most intense peak in the selected region, finds the energy of the most intense peak in that region in its database, and shifts the data to relocate the most intense peak to the energy in its database. All spectra in other regions are shifted a like amount.

The Shift function from the Auto Reduction Setup dialog box automatically performs the Shift specified in that dialog box.

*See also Shift Setup....*

## **Shift Setup...**

Selecting this function from the Data menu of the Spectrum window displays the Shift Setup... lower toolbar, and three vertical cursors are added to the display: two analysis region boundaries and a reference energy cursor. The mouse functions are summarized in Table 3-15. First, expand the region that contains the peak of interest by selecting one of the buttons in the region bar, then use this function to shift acquired data according to a reference peak energy in one of three ways:

- Press the **Auto Shift** button in the lower toolbar (or select Data–Shift). This shifts the energy of the data's most intense peak in the region to the peak energy defined in the element database for the current region, and shifts all other spectra in the current file by the same amount.

### **3: MultiPak Functions**

*Table 3-15. Mouse Functions during Shift Setup....*

To:	Point At:	Press:
Select spectra to be shifted	selection slider	(see Select Spectra)
Shift the data according to the energy shown in PkEnergy	energy cursor	Left & drag to desired location
Change the energy shown in PkEnergy	energy cursor	Right & drag to desired location

- Select one, some, or all of the spectra, then drag the energy cursor with the left mouse button to a new location (typically, a peak in the acquired data). The energy at which the mouse button is released is shifted to the energy shown in the PkEnergy field. Only the selected spectra are shifted.
- Select one, some, or all of the spectra, then drag the energy cursor with the right mouse button to a new location. The energy at which the mouse button is released is placed into the PkEnergy field. The operator then drags the cursor with the left mouse button to indicate the location on the acquired spectra that this energy should be located.

The **Undo** button undoes the last shift executed during the current session of the Shift Setup... function. The functions of the **ShowAll/ShowOne** buttons and the selection slider are described in Select Spectra.... **Cancel** exits the function without taking any action. **Exit** exits the function.

## **Shirley**

A right to left integration between the two cursors is performed generating an integrated background curve. The background type (Linear, Smart, Shirley, Iterative Shirley, or none) is specified in the Analysis Region Properties or Transition dialog box.

*See Appendix A, “Background.”*

*See also Analysis Region Properties; Transition Dialog Box.*

## **Shortcut Keys**

*See System Settings....*

## **Shrpn**

*See Filter....*

**Smart**

A right to left integration between the two cursors is performed generating an integrated background curve. The background type (Linear, Smart, Shirley, Iterative Shirley, or none) is specified in the Analysis Region Properties or Transition dialog box.

*See Appendix A, “Background.”*

*See also* Analysis Region Properties; Transition Dialog Box.

**Smon**

*See Filter...; Smooth (Binomial 3); Smooth/Derivative; Smooth/Derivative Setup....*

**Smooth**

*See Filter...; Smooth (Binomial 3); Smooth/Derivative; Smooth/Derivative Setup....*

**Smooth (Binomial 3)**

The Smooth (Binomial 3) function may be selected from the Data menu of the Profile window or the upper toolbar (Bin3) of the Profile window. (Bin3 may also be available in the upper toolbar of the Spectrum window. Refer to Smooth/Derivative Setup....)

Selecting this function causes a binomial 3-point smooth to be applied to the data selected. Doing a binomial smooth a second time to the same data is equivalent to performing a 5-point smooth. Doing a Binomial smooth a third time to the same data is equivalent to performing a 7-point smooth, etc.

*See also* Smooth/Derivative Setup...; Appendix A, “Smooth.”

**Smooth/Derivative**

Selecting this function from the Data menu of the Spectrum window performs the actions currently specified in the Smooth/Derivative Setup... function.

*See Auto Reduction Setup; Smooth/Derivative Setup....*

**Smooth/Derivative Setup...**

Selecting the Smooth/Derivative Setup... function, available from the Data menu of the Spectrum window, opens the Smooth/Derivative Setup... lower toolbar.

Smoothing reduces the noise evident in spectral data, thereby improving the visual presentation of the data and helping with data interpretation.

### **3: MultiPak Functions**

Differentiation is typically performed on AES spectra to see the relative intensities of peaks in the spectrum and remove the sloping background. Figures 3-25 and 3-26 show an AES spectrum before and after executing a 9-point Savitzky-Golay (SG) smooth and 9-point differentiate using the Smooth/Derivative function.

*NOTE: AES data that will have atomic concentrations calculated using MultiPak should have a 5-point differentiation applied **only**. Data with a 5-point smooth, matches the data used to create the relative sensitivity factors used for quantification of Auger spectra..*

*NOTE: In general, the fewer points selected for the Differentiation routine, the sharper the differentiated peak shape and the greater the resultant noise. The larger the number of points specified, the broader the differentiated peak shape and the lower the resultant noise.*

*Usually, a number between 5 and 13 will provide good peak definition and a reasonable noise level.*

The Savitzky-Golay algorithm is a polynomial function that eliminates some noise from the data and tends to preserve the peak shapes of the original data. The Binomial algorithm is a weighted average. While it is better at removing periodic noise than the Savitzky-Golay algorithm, some details of the peak shapes may be lost when using the Binomial algorithm.

To use this function, first turn Derivative on (typical for AES data reduction) or off (typical for ESCA data reduction). Then, turn SavGol (Savitzky-Golay) or Binom (binomial) on or set them both to off. Finally, in the option menu below each selected function set the number of data “points” to use. (The Derivative, Savitzky-Golay, and Binomial algorithms each use an odd number of adjacent data channels (from 3 to 25), also called points.) The algorithm is performed when the Filter button in the lower toolbar is pressed.

The Undo button can be pressed to undo the smooth/derivative action. Exit terminates the function and changes the name of the Smooth/Derivative button on the upper toolbar (e.g., S9D9, Binom3, or blank if the Deriv, SavGol, and Binom switches are all turned off).

*See also Smooth (Binomial 3).*

### 3: MultiPak Functions

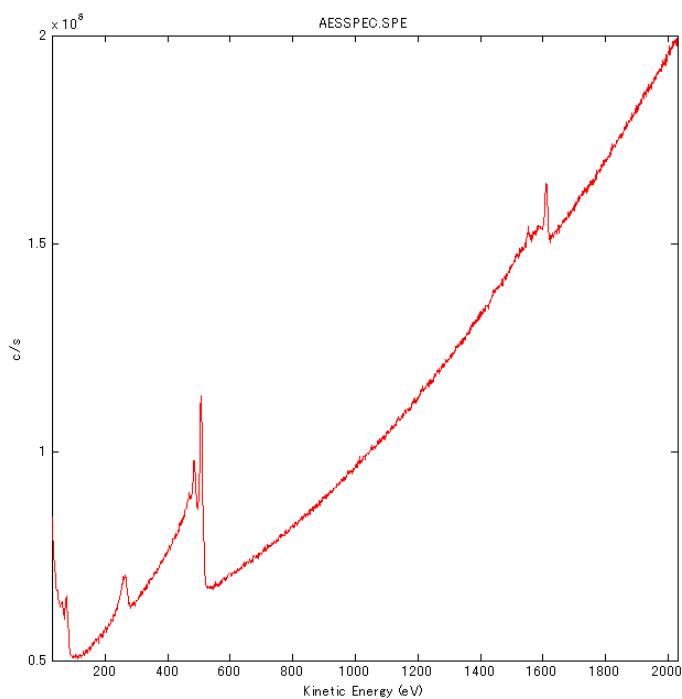


Figure 3-25. Spectrum before 9-point Savitzky-Golay Smooth and Differentiate Using the Smooth/Derivative Function.

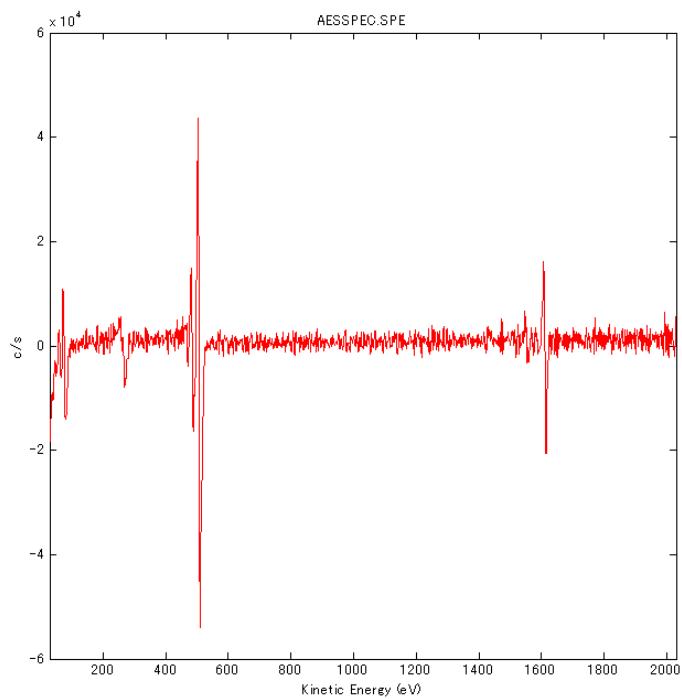


Figure 3-26. Spectrum after 9-point Savitzky-Golay Smooth and Differentiate Using the Smooth/Derivative Function.

## **SnDn**

*See Smooth/Derivative Setup....*

## **SpatArea**

*See Spatial Area.*

## **Spatial Area**

This function is available from the Tools menu (Spatial Area) of the ESCA Spectrum and Map windows and upper toolbar (**SpatArea**) of the ESCA Map windows. It is intended for data acquired on the PHI Quantera and Quantum 2000 *only*.

It displays the image from the SXI file associated with the current file, if there is one, or, if there is no SXI file, the image from the PHO file associated with the current file is displayed, if there is one. The analysis areas for the associated data file are displayed on the image.

## **Spec/New and Spec/Upd**

Pressing the **Spec/New** button creates a new spectrum from the currently selected data and establishes a direct link between the current data in the Profile or Map window and the display in the Spectrum window.

Once the link is established by pressing Spec/New, the button is renamed **Spec/Upd** (update). The button will be named Spec/Upd until a new map or profile is selected or another function is activated that breaks the direct link between the data in the Profile or Map window and the data in the Spectrum window. Pressing the **Spec/Upd** button does manually what turning on the Data Link button does automatically: It assures the user that the data displayed in the Spectrum window reflects the current data in the Profile or Map window.

*See also Data Link; Extract Spectra.*

## **Spectral Deconvolution**

This function is available from the Data menu in the Spectrum window and is used to mathematically increase the resolution of XPS peaks by removing the analyzer broadening function from the spectrum. When an XPS spectrum is measured, the widths of the various peaks are greater than their natural peakwidths due to “analyzer broadening”. The analyzer pass energy can be decreased to reduce the effects of broadening and increase the energy resolution in the spectrum, thereby, making the chemical information – peak positions, shapes, etc – easier interpret. However, reducing the pass energy also reduces the count rate; therefore, there is a limit to the practicality of this approach.

### 3: MultiPak Functions

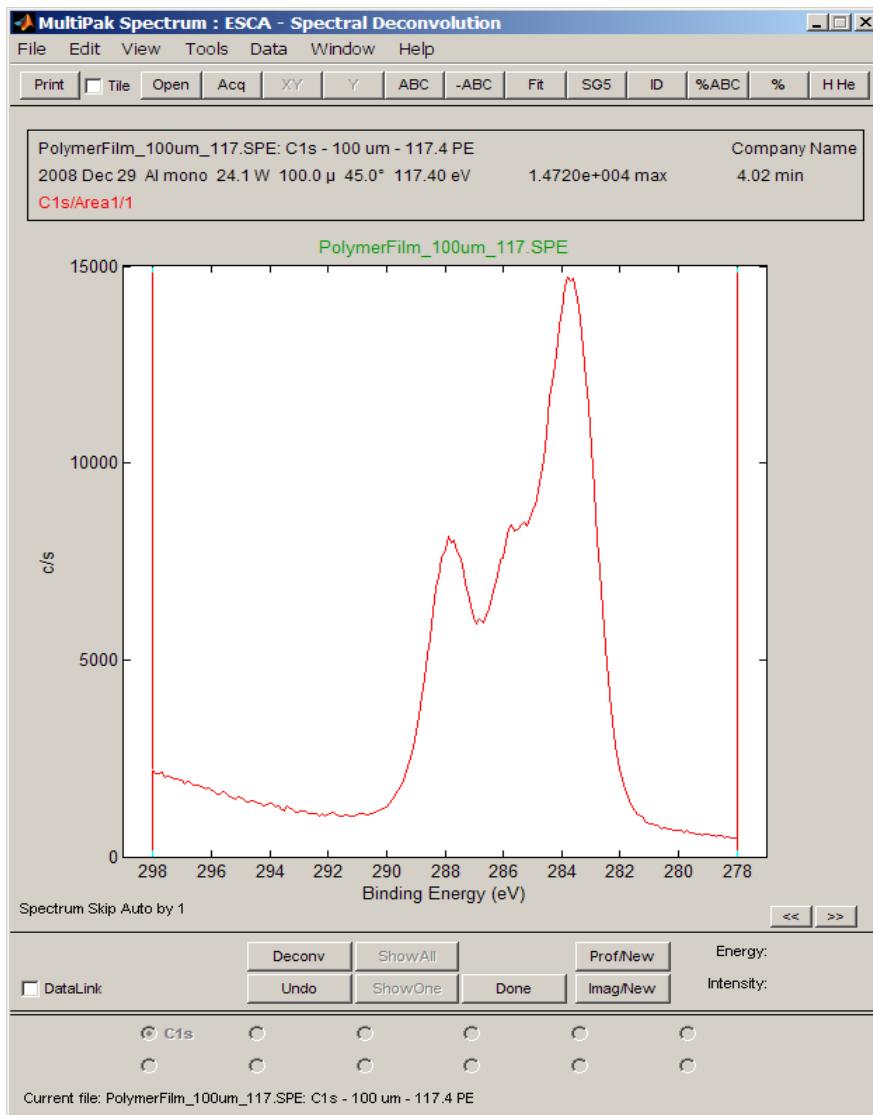


Figure 3-27. XPS spectrum in Spectral Deconvolution application.

The intended use of this function is to provide reduced measurement times and x-ray exposure for high resolution chemical analysis by XPS. To accomplish this spectra are collected at a higher pass energy where count rates are higher. The deconvolution function is then used to remove the analyzer broadening associated with the high pass energy and create spectra with the energy resolution associated with a lower pass energy. The advantages of this approach are clear: count rates will be high, data collection times will be shorter, and x-ray exposure will be reduced. For x-ray sensitive materials the lower x-ray exposure will reduce sample damage during the measurement.

The MultiPak deconvolution routine uses a set of Ag calibration spectra to remove the analyzer broadening from XPS spectra. Calibration spectra are measured according to the procedure outlined in Section 1.1. The following

steps are involved in the deconvolution procedure. The method used for deconvolution is an implementation of that described in Chapter 4 of *Deconvolution of Images and Spectra*<sup>8</sup>.

### **1.1 Measure the Ag Calibration Set**

(This procedure is normally done once for the instrument.)

Record spectra of sputter-cleaned Ag with an energy range of 372.0 – 365.0 eV using the following conditions:

1. The range of pass energies used for normal operation
2. With a data step size of 0.025 eV or the minimum step size available
3. At least 100 ms total count time per data point.

Data files must be named AgCal\_xx\_yy.spe, where xx is the instrument type – ‘QT’ for Quantera, ‘QM’ for Quantum 2000, ‘VP’ for VersaProbe I or III, ‘V3’ for VersaProbe III, and ‘5k’ for any 5000 Series instrument that does not use the focused x-ray beam technology – and yy is the integer spot size used to collect the calibration spectrum or ‘LA’ for large area (i.e., high power) mode. For example, data collected for the 20 micron beam size on a Quantera instrument would be named AgCal\_QT\_20.spe; there is one file, named AgCal\_5k\_LA.spe, required for the 5000 Series instruments.

*Note: This function is intended to be applied to data files obtained with a monochromatic Al x-ray source.*

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<sup>8</sup> Deconvolution of Images and Spectra 2<sup>nd</sup> Edition, edited by Peter A. Jannson, Academic Press, Inc., 1997, San Diego

### 3: MultiPak Functions

On/ Off	Region Name	Acquisition Lower (eV)	Acquisition Width (eV)	No. Of Sweeps	Peak/ Noise (eV)	Pass Energy (eV)	Step Size (eV)	Ratio	Analysis Lower (eV)	Analysis Width (eV)
All										
<input type="checkbox"/>	Ag3d	365.000	7.000	10	100	6.50	0.025	10	365.000	7.000
<input type="checkbox"/>	Ag3d	365.000	7.000	10	100	13.00	0.025	8	365.000	7.000
<input type="checkbox"/>	Ag3d	365.000	7.000	10	100	26.00	0.025	8	365.000	7.000
<input type="checkbox"/>	Ag3d	365.000	7.000	10	100	55.00	0.050	6	365.000	7.000
<input type="checkbox"/>	Ag3d	365.000	7.000	10	100	69.00	0.125	6	365.000	7.000
<input type="checkbox"/>	Ag3d	365.000	7.000	10	100	112.00	0.100	4	365.000	7.000
<input type="checkbox"/>	Ag3d	365.000	7.000	10	100	140.00	0.125	4	365.000	7.000
<input type="checkbox"/>	Ag3d	365.000	7.000	10	100	224.00	0.200	2	365.000	7.000
<input type="checkbox"/>	Ag3d	365.000	7.000	10	100	280.00	0.250	2	365.000	7.000

Figure 3-28. PC Compass / PHI Quantera Setting example

On/ Off	Region Name	Acquisition Center (eV)	Acquisition Width (eV)	No. Of Sweeps	Peak/ Noise (eV)	Pass Energy (eV)	Step Size (eV)	Ratio	Analysis Center (eV)	Analysis Width (eV)
All										
<input type="checkbox"/>	Ag3d	365.0	7.0	10	100	2.95	0.025	8	365.0	7.0
<input type="checkbox"/>	Ag3d	365.0	7.0	10	100	5.85	0.025	8	365.0	7.0
<input type="checkbox"/>	Ag3d	365.0	7.0	10	100	11.75	0.025	6	365.0	7.0
<input type="checkbox"/>	Ag3d	365.0	7.0	10	100	23.50	0.025	6	365.0	7.0
<input type="checkbox"/>	Ag3d	365.0	7.0	10	100	29.35	0.125	4	365.0	7.0
<input type="checkbox"/>	Ag3d	365.0	7.0	10	100	46.95	0.200	4	365.0	7.0
<input type="checkbox"/>	Ag3d	365.0	7.0	10	100	58.70	0.125	2	365.0	7.0
<input type="checkbox"/>	Ag3d	365.0	7.0	10	100	93.90	0.200	2	365.0	7.0
<input type="checkbox"/>	Ag3d	365.0	7.0	10	100	117.40	0.125	1	365.0	7.0
<input type="checkbox"/>	Ag3d	365.0	7.0	10	100	187.85	0.200	1	365.0	7.0

Figure 3-29. PC Compass / Quantum 2000 Setting example

### 3: MultiPak Functions

Active	Name	Sweeps	Pass	Lower	Range	Upper	eV Step	Ratio	P/N	Analysis Lower	Analysis Upper
<input checked="" type="checkbox"/>	Ag3d	10	6.50	365.0	7.0	372.0	0.025	10	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	13.00	365.0	7.0	372.0	0.025	8	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	26.00	365.0	7.0	372.0	0.025	8	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	55.00	365.0	7.0	372.0	0.050	6	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	69.00	365.0	7.0	372.0	0.125	6	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	112.00	365.0	7.0	372.0	0.100	4	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	140.00	365.0	7.0	372.0	0.125	4	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	224.00	365.0	7.0	372.0	0.200	2	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	280.00	365.0	7.0	372.0	0.250	2	1	365.0	372.0

Figure 3-30. SmartSoft-XPS / PHI Quantera Setting example

Active	Name	Sweeps	Pass	Lower	Range	Upper	eV Step	Ratio	P/N	Analysis Lower	Analysis Upper
<input checked="" type="checkbox"/>	Ag3d	10	2.95	365.0	7.0	372.0	0.025	8	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	5.85	365.0	7.0	372.0	0.025	8	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	11.75	365.0	7.0	372.0	0.025	6	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	23.50	365.0	7.0	372.0	0.025	6	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	29.35	365.0	7.0	372.0	0.125	4	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	46.95	365.0	7.0	372.0	0.200	4	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	58.70	365.0	7.0	372.0	0.125	2	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	93.90	365.0	7.0	372.0	0.200	2	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	117.40	365.0	7.0	372.0	0.125	1	1	365.0	372.0
<input checked="" type="checkbox"/>	Ag3d	10	187.85	365.0	7.0	372.0	0.200	1	1	365.0	372.0

Figure 3-31. SmartSoft-XPS / Quantum 2000 Setting example

	Region Name	Pass Energy (eV)	Lower (eV)	Range (eV)	Energy Step (eV)	Time/Step (ms)	Repeats
<input checked="" type="checkbox"/>	1 Ag3d	2.950	365.000	7.000	0.025	160	10
<input checked="" type="checkbox"/>	2 Ag3d	5.850	365.000	7.000	0.025	160	10
<input checked="" type="checkbox"/>	3 Ag3d	11.750	365.000	7.000	0.025	120	10
<input checked="" type="checkbox"/>	4 Ag3d	23.500	365.000	7.000	0.025	120	10
<input checked="" type="checkbox"/>	5 Ag3d	29.350	365.000	7.000	0.125	80	10
<input checked="" type="checkbox"/>	6 Ag3d	46.950	365.000	7.000	0.200	80	10
<input checked="" type="checkbox"/>	7 Ag3d	58.700	365.000	7.000	0.125	40	10
<input checked="" type="checkbox"/>	8 Ag3d	93.900	365.000	7.000	0.200	40	10
<input checked="" type="checkbox"/>	9 Ag3d	117.400	365.000	7.000	0.125	20	10
<input checked="" type="checkbox"/>	10 Ag3d	187.850	365.000	7.000	0.200	20	10

Figure 3-32.PHI-SUMMITT / VersaProbe Setting example

All calibration data files are stored in the ...\\MultiPak\\Calibration\\EnergyResolution folder. The analyst can store several sets of calibration files, if desired; the GUI for spectral deconvolution allows the analyst to specify the location of the calibration data set to be used.

#### 1.2 Run the Deconvolution function

Select the spectrum to be deconvolved. In general, the better the S/N of the spectrum, the better the deconvolution result. Enter the spectral deconvolution application, Data > Spectral Deconvolution Setup. Deconvolution is controlled by the analyst using the GUI shown in Figure 3-33; the upper panel allows the analyst to select the location of the calibration data set while the lower panel contains various parameters, described below.

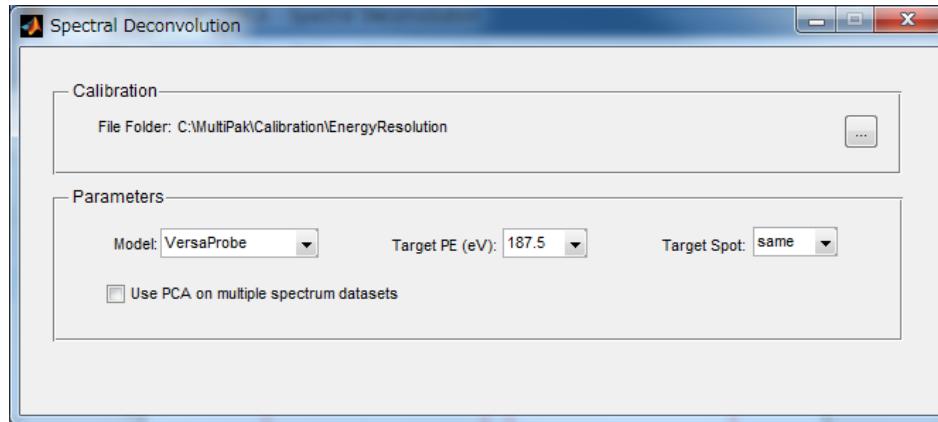


Figure 3-33. The auxiliary UI and controls for spectral deconvolution.

##### Calibration File Folder:

Indicates folder or directory to be searched for calibration files. This defaults to the folder shown in Fig. 3-33.

##### Model:

Specifies the instrument model; this selection is used to populate the Target PE (eV) list with the valid options for the instrument chosen; the instrument model stored in the data file is checked against this setting before deconvolution is performed.

##### Target PE (eV):

The pass energy for which the analyst wishes to estimate the spectrum. This should be less than the pass energy in the datafile; if not, the deconvolution request will be ignored.

**Target Spot:**

The target spot for which the analyst wished to estimate spectrum. Same option is to try to select to the same spot size of target data file, Best option is to find the best spot size for target data file.

**Use PCA on multiple spectrum datasets:**

(Multiple spectrum data sets only) Instructs the program to smooth the spectra using principal components analysis (PCA) reconstruction to improve signal-to-noise (S/N) ratio before deconvolution. This allows the low S/N spectra to be “modeled” by the stronger and the deconvolution result to be improved for spectra with lower S/N; the option is normally used with depth profile data sets where peaks may be disappearing as layers in the sample are sputtered away.

## Spectrum Skip

Spectrum Skip is a display function that can speed up the refresh rate of MultiPak’s windows when many spectra are displayed (such as when spectra from more than one profile are being displayed). Selecting Spectrum Skip from the File–Options menu in the Spectrum Window displays a cascading menu of options: Off, 2, 3, 5, 10, 20, 50, 100, Infinity, and Auto. Any selection other than Off causes only certain spectra to be displayed.

Selecting Auto allows MultiPak to choose a skip increment automatically based on the number of cycles within a region. The increment will be chosen so that not more than 20 spectra will be displayed.

Selecting 2, 3, 5, 10, 20, 50, or 100 will display only every second, third, or fifth (etc.) spectrum in each data set. Also displayed, in the lower left corner of the Spectrum window’s current data display, is a label that reads “Spectrum Skip” and the current increment.

Selecting Infinity results in the display of only the first spectrum in each data set.

Selecting Off allows every spectrum to be displayed.

*NOTE: Spectrum Skip is automatically turned off during functions like Curve Fit and Select Spectra where spectra need to be selected, then automatically restored when the function is exited.*

## Spectrum Window

*See Section 1, “MultiPak Windows.”*

## Square

*See Landscape.*

## Stack

*See Landscape.*

## Stack Plot...

The Stack Plot... function, available from the Tools menu of the Spectrum window, opens the lower toolbar so the user can automatically or interactively offset the intensities of spectra to better see the relationship between spectra. Three offset choices, illustrated in Figure 3-34, are available. When the function is started, the selection slider is turned off and the display is untiled. Settings in this toolbar are saved after closing the toolbar.

Stack plot is typically performed with the Auto button on and Overlap selected in the option menu of the toolbar. In this configuration, the offset of each spectrum is varied so the spectra overlap in the y axis but do not touch each other. When NoOver is selected in the option menu, spectra *do not* overlap in the y axis and do not touch each other. Auto mode applies offsets to the spectra in all regions of the current data.

When the Fixed button is on, the intensity offset text field of the lower toolbar is enabled and the option menu becomes disabled. In this mode, all spectra are offset by the same amount, which is defined by the user in the intensity offset field. Fixed mode applies the offset only to the current region.

The minimum data intensity of each spectrum is subtracted from the spectrum before the offset is applied.

The Reverse check box is pressed to reverse the order that the spectra of the current region are displayed. Pressing **Exit** closes the application toolbar.

## Stage Line Profiles

*See Stage Linescan; Thickness....*

## Stage Linescan

The Stage Linescan function, available from the ESCA Spectrum window’s Tools menu, makes it possible to create a line profile from peak height or peak area spectral data acquired from different stage positions. Line

### **3: MultiPak Functions**

profiles of this sort, called “stage line scans,” provide for analysis over a much larger area of the sample than can be obtained from a typical line acquisition where the x-ray beam is scanned

At each stage position, data—typically normal intensity data such as peak height or peak area—are acquired and written to a spectrum (.SPE) file.

### 3: MultiPak Functions

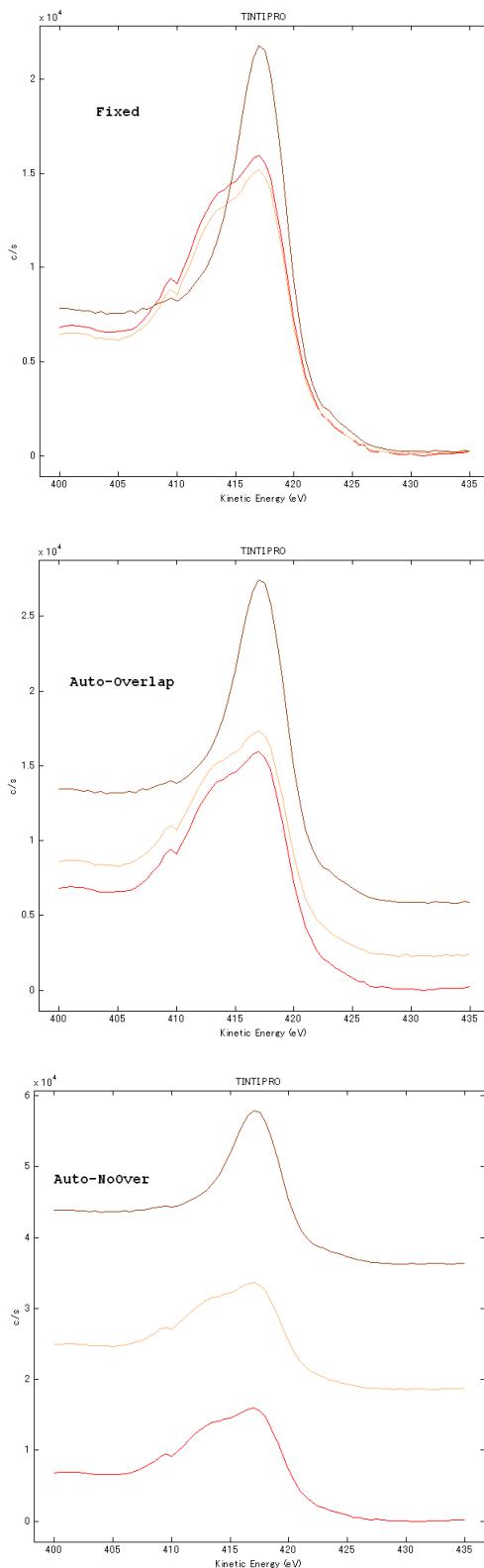


Figure 3-34. Fixed (top), Auto-Overlap (middle), and Auto-NoOver Stack Modes.

*NOTE: The same number of spectra must be present in each data file used to create a stage linescan.*

### **3: MultiPak Functions**

1. Open the spectrum files at the same time using MultiPak's Open dialog box. Overlay or New/Ovr must be checked in the lower right area of the dialog box to ensure that all files are overlaid in a single axes (plot).
2. Adjust the analysis region cursors and select the Intensity type and Background type as appropriate using the Analysis Region Properties dialog box..
3. Press the Prof/New button in the lower toolbar of the Spectrum window. A stage line profile is created for each region within the current axes, and all stage line profiles are overlaid into the same profile axis. The x axis units are distances in millimeters (mm).

*NOTE: Each spectrum file must have a unique stage position stored, all regions must have been acquired in the same order, and the files must be opened in order according to distance, since the X and Y stage positions associated with each are used to compute a distance from the first overlaid spectra to the last. These distances are used to create the x axis in the Profile window. The lower limit of the X axis is set to 0. The upper limit is set to the accumulated absolute distance (using Stage Positions) between each successive spectrum. The stage line scan function applies to Quantera and Quantum 2000 data files.*

4. If Data Link is on in the lower toolbar, the stage line profile is automatically updated after moving the analysis region cursors. If it is not on, press the Prof/Upd button in the Spectrum window to recalculate the stage line profile.

*NOTE: Once a Stage Line Profile is created its length cannot be changed.*

The beam size application is not available for Stage Linescans.

*See also* Thickness....

## **Stage Map Boundary Setup...**

The Stage Map Boundary Setup... function, available from the ESCA Spectrum window's Tools menu, makes it possible to create region maps from peak height or peak area spectral data acquired from different stage positions. Maps of this sort, called "stage maps," provide for analysis over a much larger area of the sample than can be obtained from a typical map acquisition where the x-ray beam is scanned.

At each stage position, data—typically normal intensity data such as peak height or peak area—are acquired and written to a spectrum (.SPE) file.

*See also* Thickness....

***Procedure***

1. Open the map files at the same time using MultiPak's Open dialog box. Overlay or New/Ovr must be checked in the lower right area of the dialog box to ensure that all files are overlaid in the same plot.
2. In the Spectrum window, select the analysis region from which the stage map is to be created. Then, adjust the analysis region cursors and select Intensity type and Background type as appropriate using the Analysis Region Properties dialog box.
3. Select Tools—Stage Map Boundary Setup... to define a boundary to be displayed on the stage map. (Select a boundary type (None, Rectangle, Circle/Ring, or Sector (of a circle/ring)) and parameters, and/or define a clipping boundary to eliminate a portion of the data.) A boundary is not required to create and display a stage map.
4. To create the stage map press the **Create Image** button in the Boundary Setup dialog box or press the **Imag/New** button in the lower toolbar of the Spectrum window. One map for each region in the current axis is created. The type of intensity calculation is determined by the intensity type associated with the region.

*NOTE: To create a Stage Map, the data files must contain the same number of regions and the regions must be collected in the same order and the X and Y locations must define some two dimensional shape.*

5. If Data Link is on in the lower toolbar, the stage map is automatically updated after moving the analysis region cursors. If it is not on, press the **Imag/Upd** button in the Spectrum window to redraw the map.

The current boundary definition is used to draw the boundary on the map, and, if clipping is on, data is clipped to the current clipping boundary definition.

***Boundary Setup Dialog Box***

The Boundary Setup dialog box allows the user to define a boundary shape to display on the Stage Map. In addition, the user can choose to clip (eliminate portions of) the data. The shape of the clipping boundary matches the boundary shape. The user can enter parameters to define the boundary shape and parameters to define the clipping shape. The user has four choices for a boundary shape: None, Rectangle, Circle/Ring, or Sector. The user can select the dimensions of the resulting stage map. The choices for map dimension are 64×64, 128×128, or 256×256 pixels. The original data points are interpolated to form an image of this dimension. The user can also choose to display the data points on the map that were used to create the stage map.

*NOTE: If no stage maps are associated with the regions in the current axis or there is no current axis, the Boundary Setup dialog box is set to None (the default boundary definition). If there are stage maps associated with the regions in the current axis, the Boundary Setup dialog box is set to the boundary definition associated with the stage map derived from the first region. If the Update Image button is pressed, the boundary definition is used for all regions and the stage maps associated with each region are updated.*

The Boundary Shape section of the dialog box allows the user to choose a boundary shape to be drawn on the Stage Map. The other selections vary depending on the shape selected.

In the Shape Parameter area, the **Enclose Data** button sets the Shape Parameters such that the boundary just encloses the data. The **Match Clipping** button is used to set the Shape Parameters to the values identical to the Clipping Parameters area.

In the Clipping Definition area, the user can choose whether or not to clip the data to a clipping boundary to eliminate portions of the data. Choosing Off causes the Clipping Parameter area to be disabled (grayed out). Choosing On causes the Clipping Parameter area to be enabled for defining the clipping shape.

The Stage Position Limits area of the dialog box is informational only. It shows the user the stage position limits of the data to be used in the creation of the Stage Map.

If the Display Data Points checkbox is on, the data points used to create the Stage Map are displayed on the Stage Map.

Pressing the **Save As Default** button saves the current settings as the default boundary setup to apply to all newly created Stage maps. Pressing the **Load Default** button sets the Boundary Setup settings to the last saved default values.

Pressing the **Close** button dismisses the Boundary Setup dialog box. Pressing the **Create/Update Image** button either creates Stage Maps for each region in the current axis or updates the Stage Map associated with each region using the Boundary Setup settings. Pressing the **Revert Image** button reverts any Stage Maps associated with each region in the current axis to the image prior to entering the Boundary Setup dialog box.

#### ***Rectangle Boundary with Clipping On***

Clicking on the **Enclose Data** button in the Clipping Parameter area sets the clipping vertices to the same values as the Stage Position Limits. Clicking on the **Match Boundary** button in the Clipping Parameter area sets the clipping vertices to the same values as in the Shape Parameter area.

***Circle/Ring Boundary with Clipping Off***

With the boundary shape set to Circle/Ring and the clipping option set to Off , the user enters the center of the circle/ring and an inner and outer radius. An inner radius of 0 indicates a circle. The outer radius must be greater than the inner radius.

Clicking the **Enclose Data** button in the Shape Parameter area sets the shape parameters such that the boundary is just large enough to encompass the data. Clicking on the **Match Clipping** button sets the shape parameters to the same values as in the Clipping Parameter area thus matching the clipping boundary.

***Circle/Ring Boundary with Clipping On***

With the boundary shape set to Circle/Ring and the clipping option set to On, the Center X and Center Y values for the clipping boundary are the same values as Center X and Center Y in the Shape Parameter area.

The user enters in the clipping boundary's inner and outer radius. An inner radius of 0 indicates a circular clipping shape. (The outer radius must be greater than the inner radius.)

Clicking on the **Enclose Data** button in the Clipping Parameter area sets the clipping parameters such that the clipping boundary is just large enough to enclose the data. Clicking on the **Match Boundary** button in the Clipping Parameter area sets the clipping parameters to the same values in the Shape Parameter area.

Clicking the **Match Clipping** button in the Shape Parameter area sets the shape parameters to the same values as in the Clipping Parameter area thus matching the clipping boundary. Clicking on the **Enclose Data** button in the Shape Parameter area sets the shape parameters such that the shape boundary is just large enough to enclose the data.

***Sector Boundary with Clipping Off***

With the boundary shape set to Sector and the clipping option set to Off, the user enters the center of the disk, an inner and outer radius, and a starting and ending angle. An inner radius of 0 indicates the disk has no hole in the center. The outer radius must be greater than the inner radius. The starting angle must be less than the ending angle, and both angles must be between 0 and 360 degrees. A 0 degree angle is oriented toward the right edge of the image, and angles increase counter-clockwise from that point.

Clicking the **Enclose Data** button in the Shape Parameter area sets the shape parameters such that the boundary is just large enough to encompass the data. Clicking the **Match Clipping** button sets the shape parameters to the same values as in the Clipping Parameter area..

### **Sector Boundary with Clipping On**

With the boundary shape set to Sector and the clipping option set to On the Center X and Center Y values for the clipping boundary are the same values as Center X and Center Y in the Shape Parameter area.

The user enters in the clipping boundary's inner and outer radius, and the clipping boundary's start and ending angle. An inner radius of 0 indicates the disk has no hole in the center. (The outer radius must be greater than the inner radius.) The start angle must be less than the ending angle. Both angles must be between 0 and 360 degrees.

Clicking on the **Enclose Data** button in the Clipping Parameter area sets the clipping parameters such that the clipping boundary is just large enough to enclose the data. Clicking the **Match Boundary** button in the Clipping Parameter area sets the clipping parameters to the same values as found in the Shape Parameter area.

Clicking the **Match Clipping** button in the Shape Parameter area sets the shape parameters to the same values as in the Clipping Parameter area thus matching the clipping boundary. Clicking on the **Enclose Data** button in the Shape Parameter area sets the shape parameters such that the shape boundary is just large enough to enclose the data.

### **None**

With the boundary shape set to None, no boundary shape is drawn on the Stage Map, and the data cannot be clipped.

### **Boundary Setup Dialog Box as a Stage Map Properties Sheet**

Once a stage map has been created, it is possible to modify the boundary and clipping for that stage map by displaying the Boundary Setup dialog box as a properties sheet. This is done by pressing the **Boundary Setup** button in the map's Data Properties dialog box.

Pressing the **Cancel** button cancels any changes that occurred due to pressing the **Apply** button and closes the dialog box. Pressing the **OK** button applies the changes and closes the dialog box. Changes to the dialog box while it is being used as a properties sheet affect the current map *only*; the changes do not affect the settings used when creating a Stage Map.

## **Stage Maps**

*See Stage Map Boundary Setup....*

## **Standard Annotation**

Selecting Standard Annotation from the Tools menu of the Map window places PC-ACCESS style annotation on an image. This includes the date, beam voltage/power, magnification, and a micron marker. The default font

size for annotation is used. The annotation created by this function can be moved, edited, and deleted like any other annotation in MultiPak.

## **Status Bar**

The status bar is located across the bottom of the each main window. This area displays information about the current file usually, but occasionally non-critical information for the operator can be displayed here.

## **STOP**

During file opening, a STOP button is provided in the upper toolbar for the operator's convenience. Pressing STOP prevents additional requested files from being opened. The file being opened at the time STOP is pressed will finish being opened. Pressing STOP is beneficial only when multiple files are being opened and the operator chooses not to open them all at that time.

## **Subregion**

A subregion is a subset of data from a region that can be used for further data manipulation such as LLS, spectrum extraction, line creation, etc. A subregion on a profile is defined by two subregion cursors, and on a map by a polygonal or rectangular shape. The subregion properties sheet (dialog box) can be displayed using the [Shift]-left mouse button on one of the subregion boundaries.

*See also* Region; Subregion Properties.

## **Subregion Properties**

The Subregion Properties dialog box is displayed using [Shift]-left mouse button on one of the subregion boundaries (region cursors). This dialog box shows the type of data in the subregion and the subregion's limits.

*See also* Subregion; Region Cursors.

## **System Constants**

See "System Settings...."

## **System Settings...**

The System Settings... function is available from the File–Options menu. When selected, the System Constants dialog box is displayed.

The ID field in the Miscellaneous area of the dialog box determines what MultiPak displays in the upper right corner of the header. It is set to "Company Name" as a default, and may be changed to any name 12 characters or less in length.

### **3: MultiPak Functions**

The ShowAccel ('show accelerators') toggle switch determines whether keyboard combinations (also called quick keys or hot keys) are shown next to functions listed on the menus. For example, with ShowAccel turned on, “^sc” is listed next to System Settings... in the File–Options menu, indicating that the System Settings dialog box may be displayed in one of two ways: (1) selecting System Settings... on the File–Options cascading menu, or (2) holding down the [Ctrl] key (“^”) while pressing “s” and then “c” (“sc”).

*See Appendix A, “Background,” for a description of how the Background and Number of Points fields are used.*

The axis font size is selected in the System Font field.

*See “Export To...” for a description of selecting the ASCII Format type.*

## **Table**

Selecting **Table** from the Annotate... lower toolbar displays the current settings (font, type size, etc.) for atomic concentration table annotation, allows the user to change the settings, and applies the displayed settings to the selected annotation (**Apply** button) or all annotation (**Apply All**).

Selecting Edit–Clear Annotation–Table removes any Table-style annotation from the display.

*See also Annotate....*

## **Tape Measure...**

The Tape Measure... function is available from the Tools menu of the Map window.

Once activated, dragging the mouse will create a line (or dot) and an associated number on top of the image when the mouse is released. The line is a straight line between the point where the mouse was pressed and where the mouse was released. If a horizontal or vertical line is desired, select the Constrain check box in the lower toolbar.

When the mouse button is released, a black line is displayed with a number next to its endpoint. The units of measurement for this number can be seen with the numbers listed next to the x and y axes in the lower left corner.

MultiPak stays in Tape Measure mode until the Exit button in the lower toolbar of the Map window is pressed. All Tape Measure text or lines can be dragged, edited, or deleted in the same manner as other MultiPak annotation. The result of Tape Measure is displayed with fifth place of decimals.

## **Target Factor Analysis...**

This function is available from the Tools menu of the Profile window.

### **3: MultiPak Functions**

*NOTE: The Target Factor Analysis function is available for profile data reduction only.*

The Target Factor Analysis (TFA) function is used to extract active component spectra from a set of overlapped composite spectra in a profile that are composed of varying compositions of the same number of spectral components. If used properly, it can remove some of the noise associated with the spectra (multivariate smoothing), deconvolute the overlapped spectra (multivariate curve fitting), and extract chemical profiles from the original composite profile.

Basically, two stages are involved in a typical TFA process. First, principal component analysis (PCA) is used to determine the number of component spectra that is required to reproduce the original spectral data. Note: that PCA identifies the number of spectral components needed to mathematically reproduce the original data but does not identify the actual shape of the spectral components. *Spectral* target factor analysis (SpecTFA) can be used to test suspected component spectrum from the spectral data in the profile data set or from an external basis spectrum. Once all of the component *spectra* are identified, TFA will produce profiles for the component spectra automatically. As a result of the Spec TFA fitting process some noise may be removed from the data improving the resulting profile appearance and dynamic range. Alternatively, *concentration* target factor analysis (ConcTFA) can be used to test suspected component concentration profiles supplied by the user, once all component concentration *profiles* are identified, TFA will create spectra for the component concentration profiles automatically.

Certain conditions have to be met for a successful TFA of the spectra from a profile:

- There should be enough difference in the composition of component spectra in the overlapped composite spectra from a profile. When the composite spectra in a profile come from a sample of homogeneous chemical composition or from the multiple transitions of one element (multiplet peaks), there is no difference in the composition of component spectra, and a single “composite” component spectrum will be obtained from TFA instead of the separate pure component spectra.
- If the spectra are not charged uniformly charge shifting has to be done before performing TFA, because spectra that are offset by changes in charging will introduce additional non-chemical components that cannot be tested.
- Spectral background will also introduce additional non-chemical components that can only be tested with pure background spectra. The background has to be removed if pure background spectra are not available.

### **3: MultiPak Functions**

There are five parts of the TFA routine: Profile Selection, Current Profile, Eigenvalues, Spectral Target Selection, and Concentration Target Selection. These are the names displayed in the title bar of the Profile window at different times during the routine, and correspond to the subsections of the following discussion.

The Profile window toolbar functions during TFA are summarized in Table 3-16, and the Spectrum window toolbar functions during TFA are summarized in Table 3-17.

*See also Appendix A, “Target Factor Analysis.”*

#### **Profile Selection**

When Target Factor Analysis is selected from the Tools menu of the Profile window, the title bar of the Profile window changes to read “Profile Selection.” Select a region profile in the Profile window by clicking on it or on its associated region name in the upper right corner.

### 3: MultiPak Functions

Table 3-16. Lower Toolbar Functions in the **Profile** Window during Target Factor Analysis.

Button/Check Box	Result
PCA	The title bar of the Profile window changes to “Eigenvalues,” the PCA button becomes disabled, and the SpecTFA and ConcTFA buttons become enabled. See “Eigenvalues” in this subsection.
PCASm	If the PCASm check box is checked when Exit is pressed in the TFA toolbar, all the spectra of the profiles that have PCA results are smoothed, the original spectra are replaced with smoothed spectra within the region limits, and the profiles are updated based on the smoothed spectra.
SpecTFA	The title bar changes to Spectral Target Selection. See that subsection in this discussion.
ConcTFA	The title bar changes to Concentration Target Selection. See that subsection in this discussion.
DispAll	The title bar changes to Profile Selection. Another profile may be selected at this point.
PCATable	Generates and displays a table of PCA test values. Refer to Appendix A, “Target Factor Analysis,” for a description of these test values.
SpecT	Use spectral targets for TFA
ConcT	Use concentration targets for TFA
Basic (Ext. Basis)	Displays file dialog box, retrieves a target spectrum (external basis spectrum) from a spectrum file specified by the user, displays the file name next to the current target cursor, target-tests the spectrum, and displays the target, the prediction, and the residual error in the Spectrum window.
Basic On (Ext. Basis On)	Indicates that an external basis spectrum file is to be used as a target spectrum for the current target.
DelConc	Deletes the selected concentration data point.
ClearAll	Clears all PCA/TFA results on all profiles.
ClearCurr	Clears the PCA/TFA results on the current profile.
ClearPCA	Clears the PCA results on the current profile.
ClearSTFA	Clears the spectral TFA results on the current profile.
ClearCTFA	Clears the concentration TFA results on the current profile.
Cancel	Terminates the TFA function without taking any action.
Exit	(1) If the <b>PCASm</b> check-box is checked, all the spectra of the profiles that have PCA results are smoothed, and the profiles are updated based on the smoothed spectra; (2) new component profiles are created from the TFA-resolved component spectra for the profiles that have TFA results; and (3) the TFA application is closed.

### Current Profile

When a profile region is selected at the beginning of the TFA function, the title bar of the Profile window is changed to “Current Profile,” the Profile and Spectrum windows are refreshed to show just that region, and the lower toolbars in each window also change. The curve is displayed as a solid line and in full scale. If a PCA calculation has already been performed on this profile, the PCA-reconstructed profile will also be displayed in plus (“+”) signs.

### 3: MultiPak Functions

Table 3-17. Lower Toolbar Functions in the **Spectrum** Window during Target Factor Analysis.

Button/Check Box	Result
ShowOne	Displays the middle one of the PCA-reconstructed spectra and the noise removed by PCA.
ShowAll	Displays all the PCA-reconstructed spectra and the noise removed by PCA.
SaveSpec	Saves the predicted spectrum to a spectrum file. This button is enabled when the Target button is on.
Norm	Displays normalized component spectra. The colors of the component spectra will match the colors of the component profiles displayed in Profile window.
Resolved	Displays TFA-resolved component spectra. The colors of the component spectra will match the colors of the component profiles displayed in Profile window. The coefficients (relative contribution in the composite spectrum) of the component spectra will be displayed inside the axis. Also displays the spectrum selection bar, described later in this discussion. <i>NOTE: The coefficients may not add up to 1 due the inherent noise.</i>
Target	Displays the current target spectrum and predicted spectra (transformed or projected spectrum).
Prof/Upd	(See Prof/New.)

### Eigenvalues

When the PCA button is pressed in the lower toolbar during the TFA function, the title bar in the Profile window changes to “Eigenvalues” and the PCA button becomes disabled. An eigen analysis is performed on the current profile. The logarithms of the first 25 eigenvalues are displayed in the log(eigenvalues) plot, with a vertical cursor placed between the last principal component “found” and the first error component. All principal eigenvalue data points are displayed in solid squares, and the error eigenvalue data points are displayed in outlined squares. Plots of the PCA-reconstructed spectra and the removed noise are displayed in the Spectrum window.

The operator can choose the principal components on the plot by moving the vertical cursor or clicking on the data points. When the vertical cursor is dragged, only the eigenvalues to the left of the cursor will be chosen as principal eigenvalues. Clicking on any eigenvalue toggles that eigenvalue or error eigenvalue on (principal) and off (not principal). The plots in the Spectrum window are updated as soon as the selection of components changes on the plot in the Profile window.

The horizontal cursors displayed in the PCA-Reconstructed Spectra axes can be used to select a range of spectra. Residual spectra will be updated with the PCA-reconstructed spectra.

### Spectral Target Selection

When the SpecTFA button is pressed in the lower toolbar during the TFA function, the title bar in the Profile window changes to “Spectral Target Selection” and the SpecTFA button becomes disabled. The TFA-resolved

component profiles are displayed as dotted lines whose colors match the colors of the component spectra displayed in Spectrum window. Vertical target cursors are also displayed with (1) target names (Factor 1, Factor 2), and (2) names of spectra files being used as target spectra, if the BasicOn check box is set to on.

The type of data displayed in the Spectrum window depends on which button is on in the lower toolbar of the Spectrum window:

- If the “Target” button is on, a target spectrum is displayed in the Spectrum window. For an internal target spectrum selected from the profile, the original spectrum (before PCA smoothing) and the noise removed by PCA are also displayed. For an external target spectrum from a file, the TFA-predicted component spectrum and the prediction error are also displayed.
- If the “Resolved” button is on, the TFA-resolved component spectra of one of the composite spectra are displayed, and the noise removed by PCA for that spectrum is also displayed for reference. You can display the resolved component spectra for a different PCA-reconstructed spectrum by choosing the desired spectrum using the spectrum selection bar.

You can select a different spectrum in any of the following ways (see also Select Spectra): (1) dragging the spectrum selection cursor in the selection bar, (2) clicking inside the selection bar at the position of the desired spectrum, or (3) clicking the up or down arrows in the selection bar to display the previous or next spectrum.

Along with the TFA-resolved component spectra are coefficients that represent the relative contributions of each component spectrum to the composite spectrum. (*NOTE: The noise in the spectra or the wrong choice of component spectra can cause the sum of these coefficients to not add up to 1.*)

- If the “Norm” button is on, the normalized component spectra are displayed.

To test a target against a spectrum from a different file, press the Basic button in the lower toolbar of the Profile window. The Load Target Spectrum dialog box opens, displaying the spectrum files in the “...\\datafiles\\basis” directory. When the operator highlights a file and clicks on OK, the target spectrum in that file is tested. If the external spectrum is suitable for target testing, the displays in the Profile and Spectrum windows are updated, and the name of the external spectrum file is displayed next to the current target cursor.

The name of the currently selected component spectrum in the Spectrum window is green. This is the spectrum that is saved when the SaveSpec button is pressed.

#### **Concentration Target Selection**

When the **ConcTFA** button is pressed during the TFA function, the title bar in the Profile window changes to “Concentration Target Selection” and the ConcTFA button becomes disabled.

The target labels are displayed in the upper right corner. Only one may be selected at a time. Initially, the target concentration profile has  $n+1$  “concentration data points” along the profile, where  $n$  equals the number of principal components selected. Data points can be dragged with the mouse to construct a target concentration profile. Data points may also be added to the curve by clicking the [Shift]-left mouse button at a new position within the axes, or deleted by clicking on the data point with the left mouse button, then pressing the **DelCone** button in the lower toolbar.

Whenever the number or the positions of the data points are changed, a free-float target-test is performed on the concentration points and the predicted concentration profile is updated.

The TFA-resolved component spectra of one of the composite spectra are displayed, and the noise removed by PCA for that spectrum is also displayed for reference. You can display the resolved component spectra for a different PCA-reconstructed spectrum by choosing the desired spectrum using the spectrum selection bar.

You can select a different spectrum in any of the following ways (*see also* Select Spectra): (1) dragging the cursor in the selection slider, (2) clicking inside the selection slider at the position of the desired spectrum, or (3) clicking the up or down arrows in the selection slider to display the previous or next spectrum.

Along with the TFA-resolved component spectra are coefficients that represent the relative contributions of each component spectrum to the composite spectrum. (*NOTE: The noise in the spectra or the wrong choice of component spectra can cause the sum of these coefficients to not add up to 1.*)

The name of the currently selected component spectrum in the Spectrum window is green. This is the spectrum that is saved when the **SaveSpec** button is pressed.

## **Text**

Selecting Text from the Annotate... lower toolbar displays the current settings (font, type size, etc.) for Text annotation, allows the user to change

the settings, and applies the displayed settings to the selected annotation (**Apply** button) or all annotation (**Apply All**).

Selecting Edit–Clear Annotation–Text removes any Text-style annotation from the display.

*See also* Annotate...; Clear All Annotation; Clear Annotation.

## Text Properties

The Text Properties dialog box is displayed using [Shift]-left mouse button when the mouse pointer is on top of annotation that was created by the user.

This dialog box is used to define the attributes of annotation: font, size, weight, orientation, color, marker size and marker types. The possible selections are displayed by clicking on the arrow to the right of each field. Orientation is given in angular degrees.

Settings that have been changed are applied to the selected text when the **Apply** button is pressed or saved when the **OK** button is pressed, which closes the dialog box. Pressing **Cancel** cancels any changes made since the last time the Apply or **OK** button was pressed, and the dialog box is closed.

*See also* Annotate...; Clear Annotation.

## Thermal

*See* Color Option Menu.

## Thickness...

This function, available from the Tools menu of the ESCA Spectrum window, is used to measure the thickness of a uniform thin film on a smooth surface and display the result(s) in a table or as a stage line profile or stage map. This function can only be used when the film and substrate peaks are both contained within a single acquisition region in the spectra.

When the function is started, two sets of cursors are displayed to set up two regions: one for the film material and one for the substrate material. The cursors can be dragged to the desired locations or automatically adjusted for each spectrum, depending on the state of the Automatically Adjust Regions Cursors for Each Spectrum checkbox in the Thickness Parameters dialog box. The Analysis Region Properties dialog box can be displayed using a Shift-left mouse click on one cursor to allow a user to change the Intensity calculation method (Area or Height) or the Background calculation method (Shirley, iterated Shirley, linear, or none) for each region.

After changing the parameters in the Thickness Parameters dialog box to the desired values, the results of the thickness calculation for all selected spectra can be viewed or printed in a tabular format by pressing the **View** or **Print** button in the Thickness Parameters dialog box. The format of the table can

### **3: MultiPak Functions**

be specified by pressing the **Output Setup** button to pop up the Output Setup dialog box. Several checks are done during the thickness calculation to flag possible error conditions. These checks are controlled by the Error Setup dialog box available from the **Error Setup** button and are described in detail in Appendix A. If errors are detected, they are reported in the thickness output table if the Show Error Information checkbox is selected in the Output Setup dialog box.

*NOTE: The values of all parameters and the positions of the Film and Substrate region cursors will be saved from one MultiPak session to another.*

If a thickness calculation is done on several spectra taken at different stage positions, it may also be possible to create a stage linescan or stage map to display the thickness results (see Stage Linescan and Stage Map). To create a stage linescan or stage map from the thickness results, select the **Prof/New** or **Imag/New** buttons in the Thickness Parameters dialog box. Once a stage linescan or stage map is created, the buttons change to **Prof/Upd** or **Imag/Upd**. Any time a parameter is changed, the Prof/Upd or Imag/Upd button must be pressed; there is no automatic update of the profile or map within the thickness application. Once a thickness stage map is created, it is possible to create or change the boundary setup using the Boundary Setup Properties dialog box. This

dialog box is available using the **Boundary Setup** button in the map's Data Properties dialog box.

Starting the Tools–Stage Map Boundary Setup... function during this function allows the user to change the area of the map from which spectra are used.

*Note: The Quantera SXM and Quantum 2000 data files support stage maps and line scans.*

*See also* Appendix A, “Thickness....”

## **Threshold**

*See Color Bar.*

## **TIFF**

*See Export To.*

## **Tile**

The Tile button is available from the View menu and in the upper toolbar. It toggles between displaying one (selected) large image in the window or several small images in the window. The arrangement of the display—

Landscape, Portrait, Square, or Stack—depends on the selection in the View menu.

*NOTE: Tile has no effect if there is only one file currently open.*

*See also* Landscape.

## Time

*See* Depth.

## Times

*See* Annotate...; Text Properties.

## Toggle

The Toggle button in the region bar of the Profile and Map windows turns on all the region buttons that are off and turns off all the region buttons that are on.

## Tools

The Tools menu contains functions that operate on the data (but do not modify the data). The items on this menu vary according to the MultiPak window from which the menu is opened and according to the current technique (AES or ESCA).

## Topographical Correction

The Topographical Correction function is available on the Data menu in the Profile window. It performs a normalization routine for line data that corrects for the effects of specimen topography.

*See* Appendix A, “Topographical Correction.”

## Tougaard Nanostructure Analysis...

Tougaard Nanostructure Analysis... is available from the Tools menu in the Spectrum window. Tougaard Nanostructure Analysis provides a method for determining the in-depth composition of a material by modeling the inelastic-scattering contribution to the background of an ESCA or AES spectrum.<sup>9</sup> Before starting this application, a region must be selected in the region bar in the Spectrum window.

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<sup>9</sup> For details, see:

- S. Tougaard, *Surface and Interface Analysis*, **25**, 137–154, (1997).
- S. Tougaard, *J. Vac. Sci. Technol.*, **A8**(3), 2197, (1990).
- S. Tougaard, *J. Vac. Sci. Technol.*, **A14**(3), 1415, (1996).

*NOTE: It is necessary to acquire at least 30 eV to the low kinetic energy (high binding energy) side of a peak of interest for this analysis to work properly.*

The application starts by showing the first spectrum in red, the inelastic-scattering background in green, and the result spectrum (original minus background) in blue. (If more than one spectrum is in the current plot before entering this application, select the desired spectrum using the selection slider next to the plot.) To determine the in-depth structure for a particular spectrum, adjust the parameters in the Tougaard Nanostructure Analysis dialog box until the result spectrum appears with the background completely removed.

*CAUTION: It is sometimes possible to obtain good background removal with incorrect structural parameters.*

#### **Buttons in the Lower Toolbar**

The three checkboxes—Original, Bkgd, and Result—toggle the visibility of the associated spectrum. The **SaveSpec** pushbutton can be used to save a spectrum when it is the only one visible (that is, only one of the three checkboxes is checked). The **Cancel** button exits the application without saving changes to the settings in the Tougaard Nanostructure Analysis dialog box, and the **Exit** button exits the application and saves changes to the settings.

#### **Tougaard Nanostructure Analysis Dialog Box**

The Tougaard Nanostructure Analysis dialog box allows modification of the parameters used in the analysis:

- *Inelastic mean free path*—This is specified in angstroms ( $\text{\AA}$ ) and depends on the sample composition.
- *Take off angle above the sample plane*—This is the angle of the analyzer in degrees above the sample plane. For many data files, this will be automatically set to the correct value.
- *Cross Section*—This option menu presents six inelastic scattering cross sections for different types of materials.
- *Cross section scaling factor*—This factor is used to scale the inelastic scattering background and is typically between 0.90 and 1.00, but may be slightly higher or lower.
- *Structure Model*—This option menu presents four different structure models: (1) buried thin layer, (2) exponential depth profile, (3) homogeneous depth profile, and (4) substrate with overlayer.
- *Depth*—This parameter appears only for the buried thin layer model and specifies the depth below the surface of the thin layer.

- *Decay Length*—This parameter appears only for the exponential depth profile model and specifies the depth at which the concentration goes to 0%, starting from 100% at the surface.
- *Overlayer Thickness*—This parameter appears only for the substrate with overlayer model and specifies the thickness of the overlayer.

The **Append** button adds the current parameters to the results file. The **Clear** button clears the results file. The **View** button displays the results file. The **Print** button prints the results file.

The **Cancel** button closes the dialog box without saving changes to the settings. **Exit** closes the dialog box and save changes to the settings.

## Transition Dialog Box

The Transition dialog box is displayed by clicking on an element in the Periodic Table window with the [Shift]-left mouse button. Figure 3-33 shows the AES transition Si2, and Figure 3-36 shows the ESCA transition Si2p.

This dialog box shows the values stored in MultiPak's AES or ESCA Peak ID database. The original contents of the databases, listed in Appendices B and C, includes all the transitions from PHI's XPS and AES handbooks.<sup>10</sup>

Silicon, like the majority of elements in the database, has more than one transition. The Selected and Peak Label options for each transition determine the results in the Spectrum window when (1) an element is turned on in the Periodic table window (adding options to the region bar), and (2) selecting Tools–Peak Identification, as follows:

- *Selected*—The transition is added to the region bar and included when All Transitions is selected in the Labels Option Menu. Usually, only the major transitions of an element are specified as Selected.
- *Peak Label*—The transition is added to the region bar and included when Transition Labels is selected in the Labels Option Menu. Usually, only one, the principal transition of an element, is specified as Peak Label.

*NOTE: Three additional factors also affect the result of the Peak ID function:*

- *No transitions for an element are included when that element's button is turned off in the Peak ID Setup function.*
- *Region cursors will not be displayed if the Region Cursor function is off.*

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10 K.D. Childs et al., *Handbook of Auger Electron Spectroscopy*, Third Edition, Physical Electronics: Eden Prairie, 1995; J.F. Moulder et al., *Handbook of X-ray Photoelectron Spectroscopy*, Second Edition, Physical Electronics: Eden Prairie, 1995.

### **3: MultiPak Functions**

- *No transition labels will be added to an AES spectrum if the Labels Option Menu is set to No Labels. (The Labels Options Menu is always set to Transition Labels for ESCA Peak ID.)*

One, both or neither of these switches (Selected and Peak Label) can be on or off. When Selected is turned on, the transition label (for example, Si2p) will have the prefix “s.” When Peak Label is on, the prefix “p” will be added. When both switches are on, the prefix “sp” will be added (like it is in Figures 3-35 and 3-36). The prefixes are followed by a dash and greater-than sign (->).

All values in the dialog box may be changed by the user. The user also has the ability to define new transitions or delete existing transitions. Once the **UpdDbase** (update database) button is pressed, the changes entered will be saved

When selecting the AES database file had the relative sensitivity factor values of both CMA and SCA, AES\_CMASCA.EDB or AES\_CMASCA\_AMRSF.EDB , the pull-down menu is displayed on Sensitivity Factor panel to switch either CMA or SCA. Switching either CAM or SCA user can edit or confirm the value of relative sensitivity factor with respective analyzer.

When selecting the AES database file that has only CMA’s relative sensitivity factors, the pull-down menu to switch either CMA and SCA is not displayed. An SCA’s relative sensitivity factor is converted based on CMA’s ones in each calculating atomic concentration. User can edit and confirm the values of CMA’s relative sensitivity factors in Transition Dialog Box, but note that SCA’s ones are interacted closely with CMA’s one.

### 3: MultiPak Functions

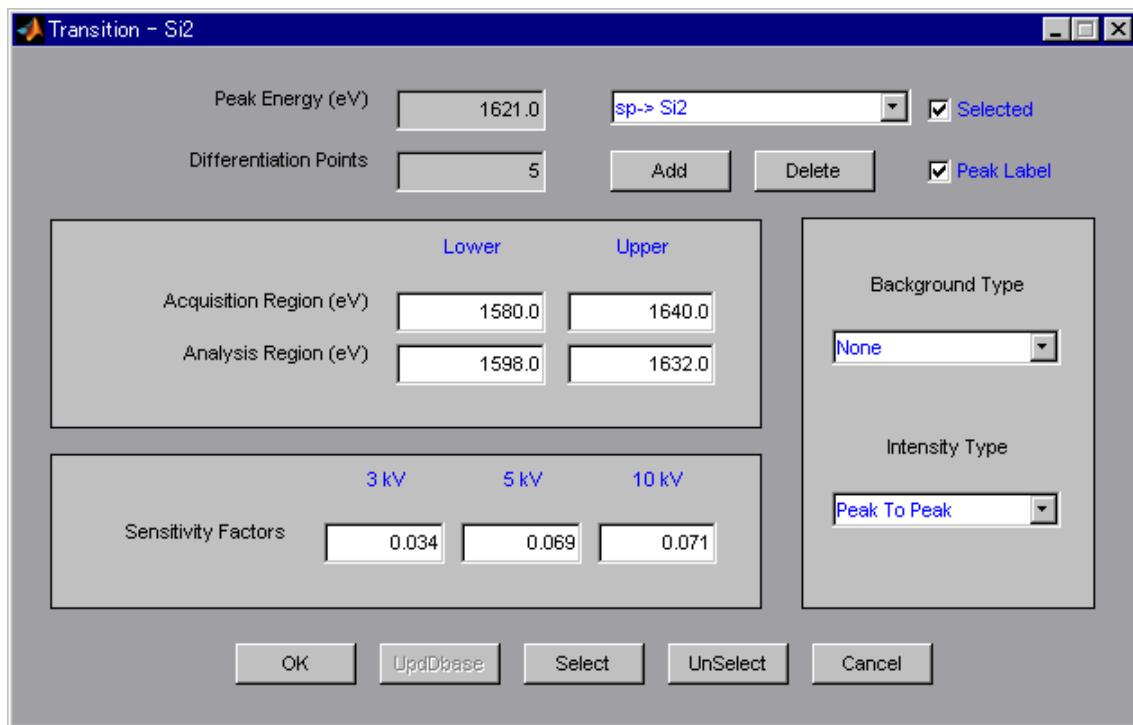


Figure 3-35. Transition Dialog Box for the AES Transition Si2.

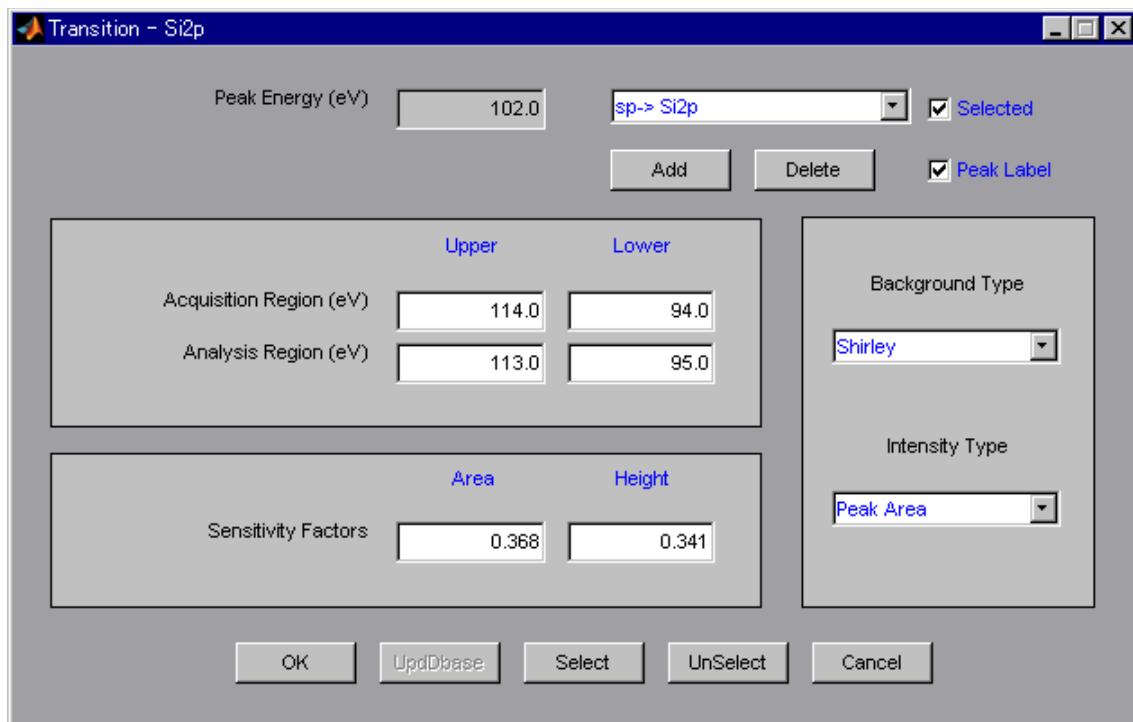


Figure 3-36. Transition Dialog Box for the ESCA Transition Si2p.

permanently to the database (until changed again). When UpdBbase is not pressed, the changes entered will be in effect only for the current MultiPak session.

### **3: MultiPak Functions**

Pressing the **Select/Unselect** buttons in the dialog box toggles the element button in the Periodic Table.

*See also* Peak Identification; Periodic Table; Regions; Appendix A, “Sensitivity Factors.”

## **Transition Label**

*See Labels Option Menu.*

## **Undo**

Selecting Undo from the Edit menu or upper toolbar of the Map window closes and reopens the current map. (File–Close and Reopen closes and reopens all open maps.)

*See also* Filter....

## **Update File**

*See Intensity Calibration.*

## **Ultra Thin Film Analysis**

### ***Overview of Ultrathin Film Analysis Functions***

There are two functions “Structure Analysis” and “SiON Depth Profile” in the Ultrathin Film Analysis (UTFA) menu which use the information about ARXPS (angle-resolved XPS measurements) to estimate in-depth sample composition versus depth non-destructively. “Structure Analysis” provides estimates of the thickness and composition of layered material from measurements at 2 angles. The (analyzable) total thickness above the substrate is limited by electron signal attenuation to roughly 4 - 5 nm. “SiON Depth Profile” allows the analyst to estimate the nitrogen distribution in silicon oxynitride films that range in thickness from about 0.5 to 4 nm. “SiON Depth Profile” is based on the assumption that the film composition is stoichiometric. Both functions require some prior knowledge, if more precise information is necessary. “Structure Analysis” is more broadly applicable. However, the information is less detailed than that from “SiON Depth Profile”.

The estimation of depth distributions or sample structure from ARXPS spectra is rather difficult work because of the low information content of the measurements<sup>11</sup>. (In principle the process to estimate the sample structure or depth distribution from ARXPS is influenced by the quantitative error of atomic concentration or noise.) The signal versus depth information is integrated over the entire sampling depth at each angle. Therefore, the

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11 See, for example, P. J. Cumpson, *J. Electron Spectrosc. Relat. Phenom.* **73**, 25(1995)

variation in signal with measurement angle can be small. It is effective for the calculation to use (1) prior information on sample structure and composition, and (2) reasonable assumptions for the stability of calculations. In principle, it is very hard to detect a small amount of an element or to calculate absolute values of thickness or concentration. However, it is fairly easy to identify the remarkable relative differences among samples.

### **Structure Analysis**

This function estimates the layer structure of thin films using spectra measured at two different “take-off angles” (TOA: angle between surface plane and input lens axis). Both the accuracy and the precision of the spectral peak intensities are important for the calculation. Note that it is difficult to estimate the layer structure when the difference in peak energies is large for the peaks being used in the calculation.

The data are collected in either SPE or ANG files; an example of the data collection conditions is given for SiON films in SiON Data Collection which is shown later in this section. To obtain the attenuation length of electrons used in the film thickness calculation, the 3/4power law of kinetic energy of electrons for IMFP calculations is applied.

The dataset should contain a high ( $80^\circ - 90^\circ$ ) and a low ( $\leq 20^\circ$ ) TOAs and is analyzed as follows.

1. Use Select File/Open in the MultiPak Spectrum window and highlight either an ARXPS (ANG) file or a group of multiplex (SPE) files containing data measured at two or more TOAs. If using SPE files, set the Spectrum Display mode in the Open menu to Overlay; click the [Prof/New] button immediately after opening the set of SPE files to establish the profile display.
2. Calculate the intensities of species from the measured spectra at the various take-off angles (TOA).

The relevant peak area intensities are determined in the standard way by adjusting the analysis region cursors for each element; the spectra may be smoothed if there is significant noise. Curvefitting may be used to separate chemical states if it is necessary.

For example, in the case of Si from a  $\text{SiO}_2/\text{Si}$  thin film structure, curvefit is used to obtain the intensities of  $\text{Si}^0$  and  $\text{Si}^{4+}$  from Si2p spectra. – the recommended procedure to fit the Si2p spectra is given in the Si Curve Fit Procedure section.

3. Update the calculated intensities in the Profile window by clicking [Prof/Upd] in the Spectrum window lower tool bar. This will move the Si curvefit results into the Profile window and allow them to be included

in Structure Analysis results. At this point the original Si2p region should be turned off and excluded from the Structure Analysis results.

4. Select the *Ultrathin Film Analysis/Structure Analysis* function in the Profile window *Tools* menu. The Structure Analysis and Structure Analysis-View windows shown in Figure. 3-37 are displayed. The number of layers and their compositions are determined from the input data. Layer 1 is always assigned as the substrate and the software shows the thickness of substrate as 8 nm, to indicate the substrate is very thick.
5. The structure automatically estimated by the program may be modified based on the user's prior knowledge of the sample.

The buttons in the Structure Analysis window are used to add or delete the layers. The chemical character – metal (or elemental), compound, organic – of each layer is specified by the pull-down menu. The species contained in each layer can be changed using the check boxes. [Auto] recalculates the structure based on the new input data.

6. A certainty of calculation layers is shown as [residue] on the Structure Analysis-View window. A smaller [residue] value suggests more certainty.
7. [Print] prints the calculation results, and [ClipBoard] places the graphical result on the Windows clipboard for transfer to other applications. [Summary] places the results into a text file.

### 3: MultiPak Functions

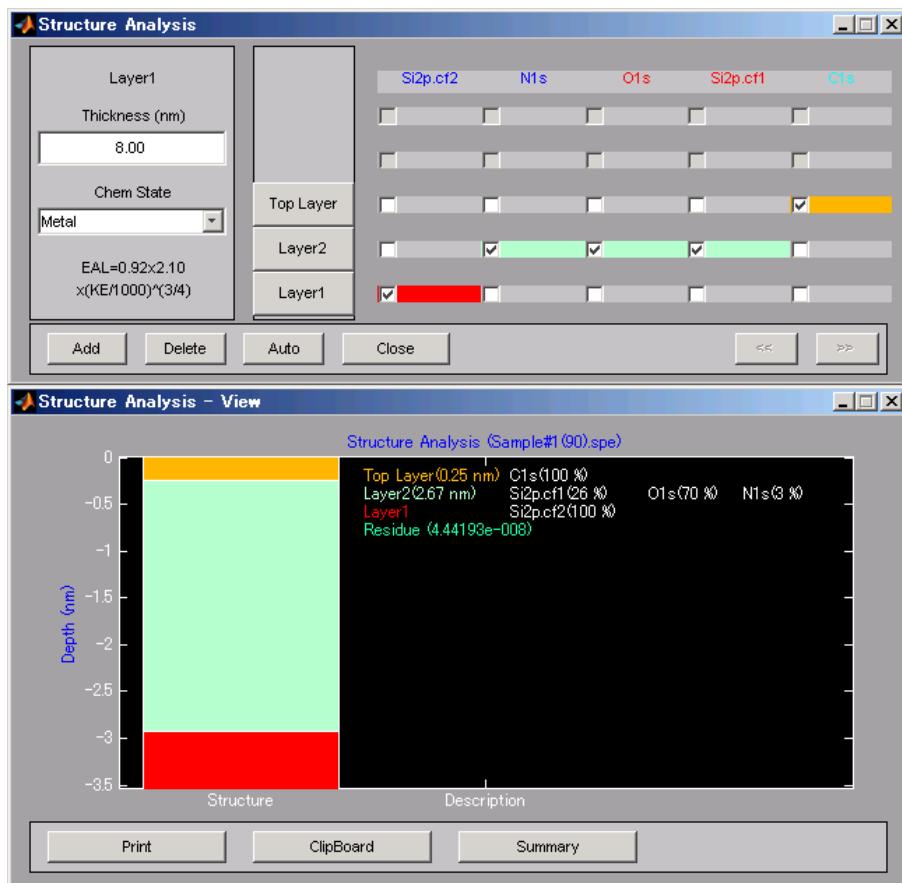


Figure. 3-37 Structure Analysis main window showing layer and composition controls (Top). Graphical view of the calculated film stack structure (Bottom).

See also Appendix A, “Ultra Thin Film Analysis.”

#### **SiON Depth Profile**

This function attempts to estimate the depth distributions of total O, total N, Si<sup>0</sup>, and Si<sup>4+</sup> species in SiON films. Both accuracy and precision of the peak intensities are important for the calculation.

The data should be collected in either SPE or ANG files as described in SiON Data Collection shown in later section. The calculation example will be shown using a typical data set.

1. Select File/Open in the MultiPak Spectrum window and highlight either an ARXPS (ANG) file or a group of multiplex (SPE) files containing data measured with recommended conditions. If using SPE files, set the Spectrum Display mode in the Open menu to Overlay; click [Prof/New]

### 3: MultiPak Functions

button immediately after opening the set of SPE files to establish the profile display.

2. Calculate peak intensities from the spectrum at various take-off angles (TOA).
  - a. Use the MultiPak curvefit function to obtain the  $\text{Si}^0$  and  $\text{Si}^{4+}$  intensities from the Si2p spectra – the recommended procedure for curve fitting of the Si2p spectra is given in the Si Curve Fit Procedure later in this section.
  - b. The O and N area intensities are determined in the standard way by adjusting the analysis region cursors for each element; these spectra may be smoothed to reduce noise in the data.
3. Update the calculated intensities in the Profile window by clicking [Prof/Upd] in the Spectrum window (lower tool bar).
4. Select *Ultrathin Film Analysis/SiON Depth Profile* function from the Profile window Tools menu,. The SiON Depth Profile window shown in Figure 3-38 is displayed. The ‘x’ symbols indicate the measured ratio of [N] to [O] at each TOA. Click [Convert] to initiate the calculation of the depth profiles for N, O,  $\text{Si}^0$ , and  $\text{Si}^{4+}$ . After the calculation, the solid line in Fig. 3-38 indicates the [N] to [O] concentration ratios that would be expected from the estimated profiles. The Film Thickness is displayed in nm and the RMS value shows the root mean square difference between the measured and calculated N/O ratios. The profiles for the four species are displayed in the Profile window as shown in Figure 3-39.

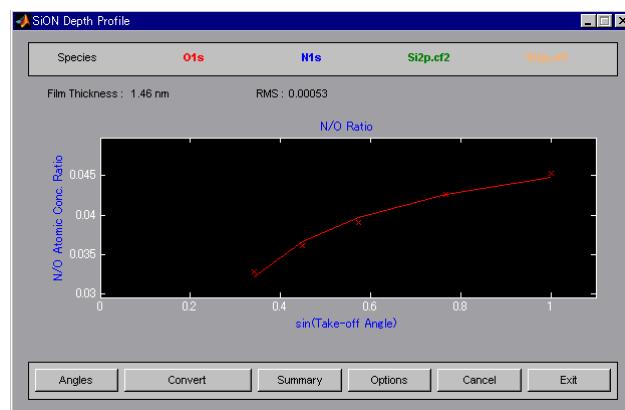


Figure. 3-38 SiON Depth Profile window. The ‘x’ symbols show the measured ratios of O and N intensities at each TOA. The solid line shows the calculated ratios used to obtain the calculated profile result.

### 3: MultiPak Functions

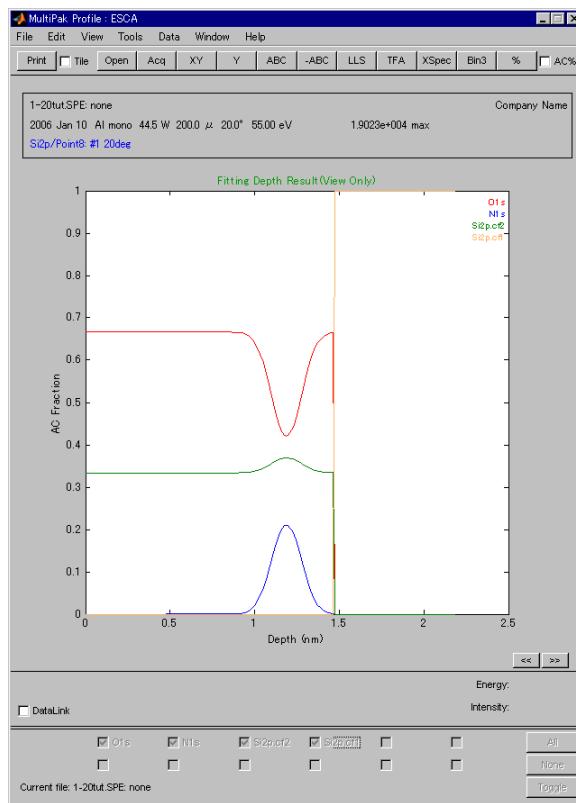


Figure. 3-39 MultiPak Profile window showing results of the SiON Depth Profile calculation.

5. If the calculation fails to converge, a window indicating this failure will appear. Since there is currently no correction for elastic scattering or for peak noise, one option is to remove the lowest angle, where elastic scattering has the greatest influence, from the calculation and try the calculation again. Click [Angles] to bring up the angles menu. Selected angles are shown in red and deselected angles in black. By clicking the button for an angle the status can be toggled from selected to deselected.
6. [Options] displays the parameter window (Figure 3-40) which contains the adjustable parameters used in the calculations. It is not necessary to modify these parameters for the most SiON calculations.
7. [Summary] shows a table of the results and lists the depth profile of the species in a text file.

### 3: MultiPak Functions

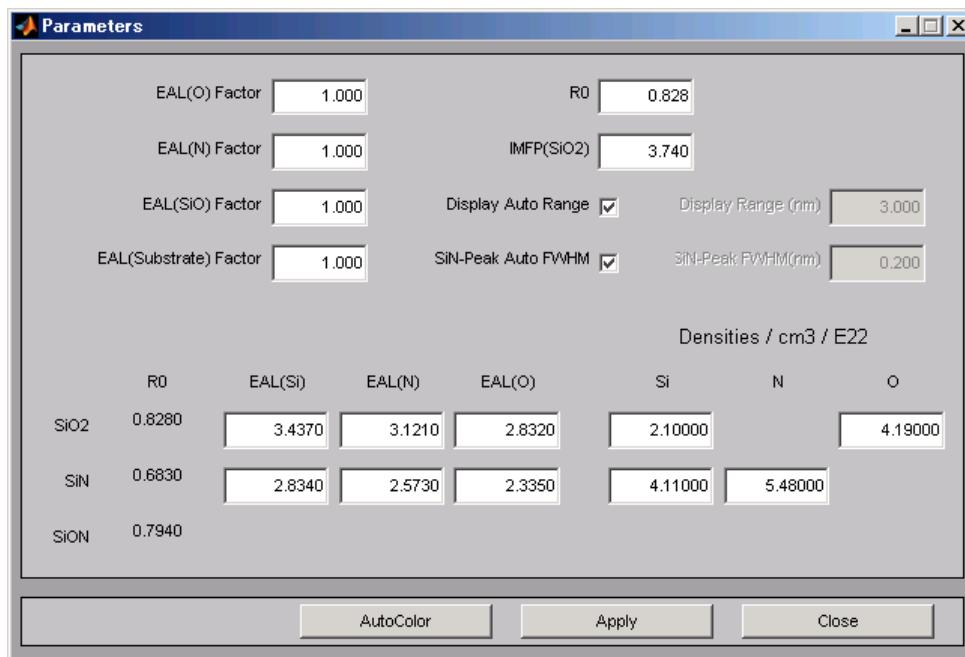


Figure. 3-40 SiON Depth Profile Parameters menu. This is displayed by clicking the Options button.

#### SiON Depth Profile Parameters Menu

The parameters (effective attenuation length (EAL) and etc.) for the calculation of SiON Depth Profile are explained. These parameters have been experimentally optimized and should not need to be changed.

##### Upper Part

- **R0** – the ratio of sensitivity factors of Si<sup>4+</sup> and Si<sup>0</sup> used in the estimate of total film thickness using the intensity attenuation.
- **IMFP(SiO<sub>2</sub>)** – the inelastic mean free path of Si 2p in SiO<sub>2</sub>; this value can be calculated from the TPP-2M expression<sup>12</sup>. The IMFP is the average distance traveled by an electron in the solid between inelastic collisions.
- **EAL (O,N,SiO,Substrate) Factor** – the value obtained by multiplying EAL by this factor is used for the calculation. If it is necessary to change EAL for the calculation, EAL can be set to the original value by changing this factor (Factor = 1.0).
- **Display Auto Range** –when unchecked, user is allowed to set total depth range for display.
- **SiN-Peak Auto FWHM** –When checked the FWHM of the profile curves is set to 0.2 nm. When unchecked, FWHM of the profile curves is user adjustable.

<sup>12</sup> S.Tanum, C.J.Powell and D.R.Penn, Surf Interface Anal. 21,165(1994)

### 3: MultiPak Functions

#### Lower Part

- **R0** – values are the equivalents of *RO* above for the different materials.
- **EAL(Si,O,N)** – the effective attenuation length (precise explanation is given by ISO 18115) is the attenuation length of photoelectrons including other effects than inelastic scattering. This value depends on the film thickness and composition. The conversion factor between IMFP and EAL is defined as 0.922.
- **Densities** – the atomic densities of the species in each material.

#### **An example of Data Collection for SiON Depth Profile**

In Table 3-18, recommended data collection conditions for the SiON structure and depth profile analyses are shown. If SPE files are used, make sure to run the [Auto-Z] routine before each acquisition.

The acquisition time for Si 2p at 90 degrees TOA is set longer than the 20 degree data because the 90 degree data will be used to determine the thickness of the film. The signal-to-noise ratio of the O and N has a significant impact on the SiON Depth Profile calculations, so it is important to spend the time needed to obtain good quality O and N spectra.

Table 3-18. Data collection conditions recommended for SiON sample.

Beam diameter : 200 $\mu\text{m}$  X-ray power : from 40 to 50 W

Species	Pass Energy	Step Size	Energy Range	time per step at	time per step at 20
---------	-------------	-----------	--------------	------------------	---------------------

	(eV)	(eV)	(eV)	90 deg (s)	deg (s)
N1s	224	0.2	542-522	0.3	0.9
O1s	224	0.2	410-390	2.0	6.0
Si2p	55	0.1	112-95	1.8	0.5

### ***Si Curve Fit Procedure***

The UTFA function requires intensities for Si<sup>4+</sup> and Si<sup>0</sup> to estimate the depth profiles from ARXPS data. The method to estimate these intensities is described in the Curve Fit section of this user guide.

In this example, Si2p measured at 55eV of pass energy(PE) with a Quantera will be analyzed by three band curvefit.

1. Select the Si2p region in the Spectrum window. Adjust the analysis window cursors to enclose the region from ~106.5 to 97.5 eV as shown in Figure. 3-41. Select the Curve Fit command from the Tools menu in the Spectrum window.
2. Check [Setup], and open [Curve Fit Setup] If Si2p spectra for an SiON dataset were previously curvefit, the appropriate bands<sup>13</sup> will be loaded from the settings file. In this case, skip to Step 3 since most of the setup has been completed. If a previous setting is not available use the following method.
  - a. Choose [Asymmetric] and [Shirley] from the pull-down menu at right corner in the setup window, hold the right mouse button down to drag and drop a band on the Si2p<sup>3/2</sup> metal (Si<sup>0</sup>) peak. Drag and drop a second band roughly at the position of the Si2p<sup>1/2</sup> metal peak. The position and intensity of this peak will be modified later.
  - b. Adjust the synthesized peak parameters to fit original peak. In this case, (1) Area Lock of band2 in curvefit setup window is set to 1, and Area ratio is set to 0.5, (2) Pos Lock is set to 1, and Separation is set to 0.63, (3) FWHM-Lock is set to 1, and FWHM Difference is set to 0.
  - c. In the MultiPak spectrum window, click and drag the position and width of band three to fit the original data for Si<sup>4+</sup>.
  - d. Adjust the Tail Length range from 5.00 to 20.00 and *Tail Scale* range from 0.0 to 3.0 in the *Band Limits* menu. In the Spectrum window, click [Fit] to fit the composite angle spectrum. The curvefit result is shown in Figure.3-41.

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<sup>13</sup> Note that the synthetic peaks are referred to as “bands” in MultiPak.

### 3: MultiPak Functions

3. Confirm that the fitting is successful. If not, repeat Step 2 to improve the fit. Save the fitting parameters in a setting file (File menu in the Curve Fit Setup window) for future use. Example parameter sets are shown in Figure 3-42.
4. Uncheck *Setup* in the MultiPak Spectrum Window, and click [Fit] to fit the individual spectra at each TOA. To confirm the successful fit of each Si2p spectrum, select [ShowOne] and use the up and down arrows to scroll through the spectra. Once satisfied, click [ShowAll] and then [Prof/Upd] to transfer the intensities to the Profile window. Exit the Curve Fit function.

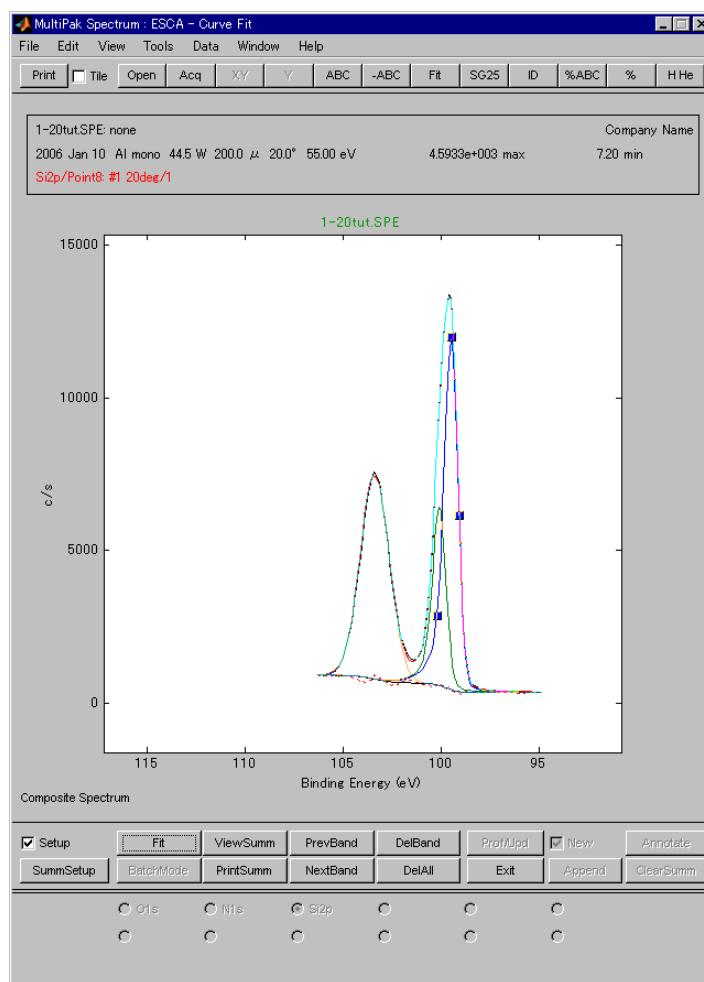


Figure. 3-41 The Si2p region curvefit for SiON Depth Profile or Structure Analysis functions.

### 3: MultiPak Functions

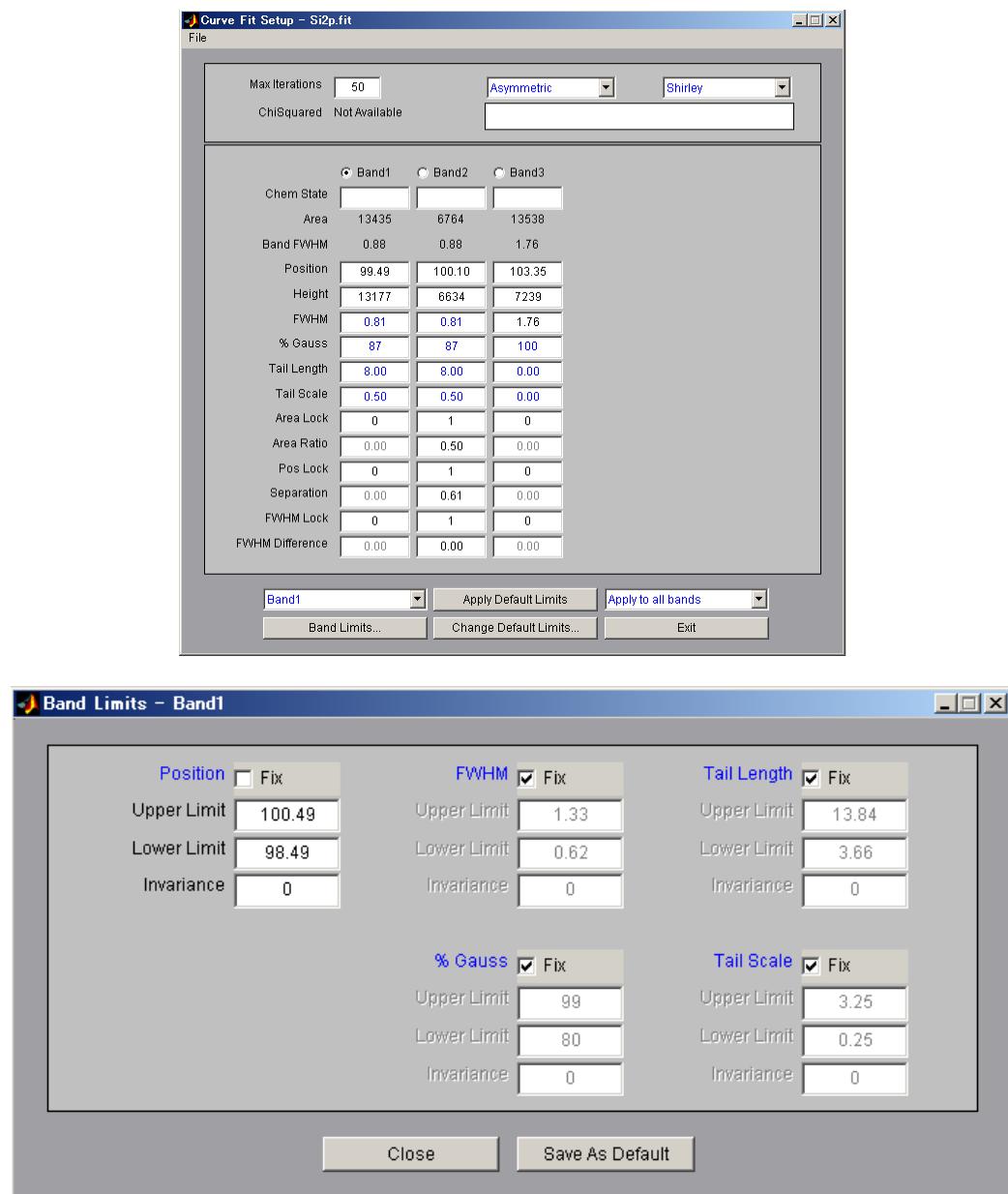


Figure. 3-42 Typical Curve Fit Setup menu after fitting a set of SiON spectra. Note that Band 2 is locked to Band 1 and the intensities will be added together in the profile display window.

### 3: MultiPak Functions

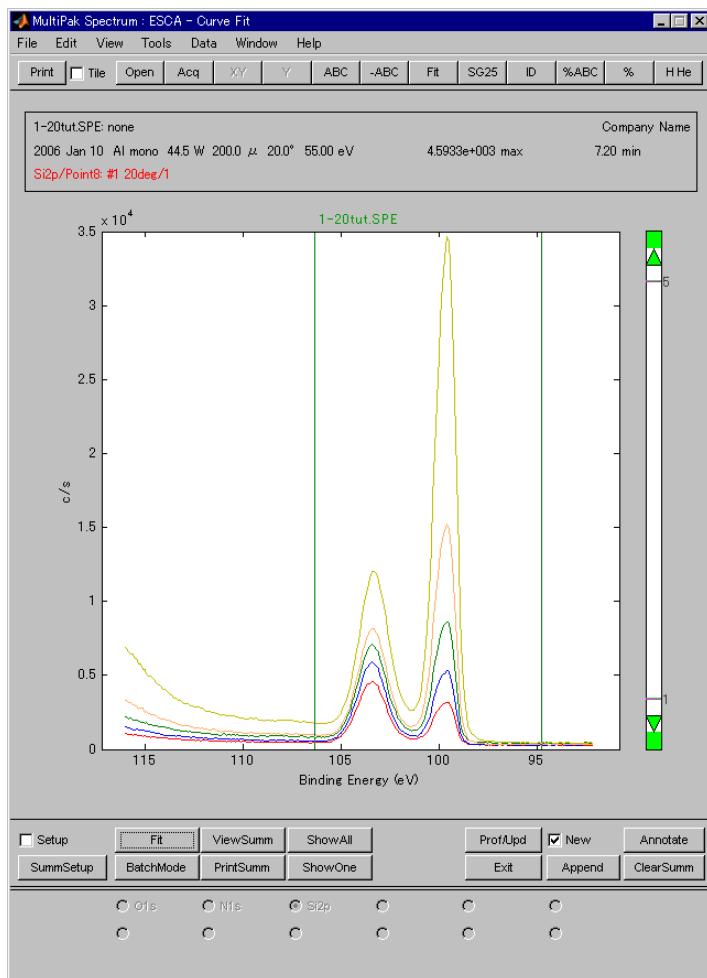


Figure. 3-43 Si 2p spectrum window showing the region cursors.

## View

The View menu of the Spectrum, Profile, and Map windows contains operations that change the data display (but not the original file). The functions listed vary according to the window from which the menu was opened. The View menu also lists other regions or files available for display and can be selected from this menu for convenience.

The View menu of the Periodic Table window lists three functions: Analysis Region, Peak ID, and Autoreduction. Refer to the discussions of those functions in this section of the manual.

Refer to “Atomic Concentration Table” earlier in this section for a description of the View function on the Atomic Concentration Table submenu.

## **White**

*See Annotate....*

## **Window**

The Window menu contains operations that affect the MultiPak windows themselves, such as Full Screen, Arrange All, and Hide MultiPak. Any of MultiPak's windows may be brought to the front of the desktop's display using this menu.

## **X-Axis Scale**

Selecting  $\mu\text{m}$ , nm, Å, s, or min from the View menu of the Profile window specifies the units of the depth scale (x axis) of data in the Profile window: microns or micrometers ( $\mu\text{m}$ ), nanometers (nm), angstroms (Å), seconds (s), or minutes (min). It will stay at this setting until changed again and will affect other profiles being opened.

If the profile being opened provides time data *only* (without defining a correlation between time and depth), the x-axis scale will be time (minutes) even when the View menu specifies depth ( $\mu\text{m}$ , nm, Å, s, or min).

*NOTE: X-axis units cannot be changed for AES line scans or ESCA angle-dependent profiles.*

*See also* Depth Calibrate.

## **XLine**

*See Extract Lines....*

## **XSpec**

*See Extract Spectra....*

## **XY**

*See Full Scale.*

## **Y**

*See Full Scale.*

## **Zoom**

The Zoom cascading menu is displayed from the View menu of the Spectrum and Profile windows. The Zoom functions allow the user to examine any part of the spectrum in as much detail as desired.

### **3: MultiPak Functions**

Zoom *In* and Zoom *Out* expand and reduce, respectively, the size of the spectrum to show smaller ranges or bigger ranges of the current spectrum within the same area of the window. The level of zoom is then maintained as the user pans right and left to view other portions of the spectrum.

*See also* Full Scale; Pan.

# Appendix A: Algorithms

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This appendix briefly describes certain mathematical algorithms for data reduction used in MultiPak. They are presented in alphabetical order for the user's convenience:

- Atomic Concentration,
- Background,
- Curve Fit,
- Differentiation,
- FWHM,
- Linear Least Squares Fit,
- Peak Area,
- Peak Height,
- Peak to Peak,
- Satellite Subtract,
- Sensitivity Factors,
- Smooth,
- Structure Analysis
- Target Factor Analysis,
- Thickness,
- Topographical Correction.

## Atomic Concentration

The atomic concentration (AC) calculation provides a ratio of each component to the sum of the other components in the data. It is displayed as a graph and/or table that illustrate the percentage or intensity of each component relative to the other components as a function of energy, time, angle, or depth.

The mathematical calculation is given as:

## A: Algorithms

$$\text{Percentage for element } x = \frac{\frac{I_x}{S_x T_x}}{\sum_{i=1}^n \frac{I_i}{S_i T_i}} \times 100 \quad (1)$$

where:

n	number of regions,
I	intensity,
S	sensitivity factor (see “Sensitivity Factors” later in this appendix),
T	acquisition time per data point.

Intensity is calculated according to the parameters in the Analysis Region Properties dialog box. That is, the intensity of AES data is calculated by (1) performing a 5-point\* differentiation; (2) normalizing the data by volts per second; and (3) computing the peak-to-peak amplitude. The intensity of ESCA data is the calculated peak height or peak area after the background is subtracted.

## Background

MultiPak calculates background using one of three algorithms: linear , Smart, Shirley, and iterative Shirley.

In all four routines, the endpoints of the background curve start at the x values of the data at the two analysis region boundaries. The boundaries should be dragged to their most appropriate positions for the most meaningful results. Then, the endpoint y values are calculated by averaging or smoothing a number of points around each region boundary.

The default is to average three points around each region boundary. The algorithm (average or smooth) and the number of points to use can be changed in the System Settings... function, which is available on the File menu of the Spectrum window.

*See also Appendix A, “FWHM/Area....”*

### **Linear Background**

A straight line is drawn between the endpoints to form the background.

For background subtraction, at each data point the value of the background curve is subtracted from the value of the data curve.

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\* The original AES database specifies this value for each transition as 5, but it can be changed (temporarily or permanently) by the operator in the Transition dialog box.

## A: Algorithms

### Smart Background

Smart Background is computed by Iterated Shirley Background, generating the background curve so that the final spectrum is non-negative.

### Shirley Background

A Shirley background helps eliminate contribution to the data from the scattering of low-energy electrons.

A right-to-left integration between the two endpoints is performed, generating an integrated background curve. This new curve is then adjusted so the amplitude of each endpoint corresponds to the amplitude of the corresponding data points in the original curve. Only positive amplitudes of the final curve are recorded and displayed, and the result is used to separate the peak from its background.

### Iterated Shirley Background

The Iterative Shirley (IterShirley) background is computed by performing the Shirley background routine five successive times for the final result. Each iteration uses the previous iteration's background as its background.

## Curve Fit

The following is a description of the nonlinear least-squares optimization procedure used to perform the automated curve fitting routine in MultiPak.\*

To begin, a set of experimental data points  $Y_i$  ( $i = 1, 2, \dots, n$ ) have been obtained at energies  $X_i$  ( $i = 1, \dots, n$ ). A function is to be defined to fit this data.  $P$  is defined as a parameter set that will contain a number of data points  $P_j$  ( $j = 1, \dots, m$ ) that define a synthetic peak structure. The purpose of the program is to find values for the parameters that give the best representation of the experimental data.

“Best” representation is defined as the set of parameter values  $P_j$  that minimizes the chi-squared value ( $\chi^2$ ) in the following equation:

$$\chi^2 = \frac{1}{n - m} \sum_{i=1}^n W_i [F(X_i, P) - Y_i]^2 \quad (2)$$

where:

- n        number of data points in the data set,
- m        number of parameters defining the synthetic peak structure,
- $W_i$     a weighting factor (defined as  $1/Y_i$ ),
- $F(X_i, P)$  function defined below,
- $Y_i$       electron intensity.

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\* The theoretical basis of this algorithm is described in “Applications of Stepwise Regression to Nonlinear Estimation,” R.I. Jennrich and P.F. Sampson, *Technometrics*, **10**:1, February 1968.

## A: Algorithms

The function  $F(X_i, P)$  is of the form:

$$F(X_i, P) = \sum_{k=1}^{n_b} B_k(X_i, Q) \quad (3)$$

where:

- $n_b$  number of bands used to define the synthetic peak structure,
- $B_k$  the function defining a single band,
- $Q$  the parameters in the function to define the band.

The parameter set  $P$  will, therefore, be the union of the parameter sets  $Q$  for each of the  $n_b$  bands.

The curve fitting routine allows three forms of  $B(X_i, Q)$ : Gaussian, Gaussian-Lorentzian, and Asymmetric Gaussian-Lorentzian, as follows:

- **Gaussian:**

$$B(X_i, Q) = H \cdot e^{-\ln(2) \left[ \frac{2(X_i - PP)}{FWHM} \right]^2} \quad (4)$$

- **Gaussian-Lorentzian:**

$$B(X_i, Q) = H \left\{ PG \cdot e^{-\ln(2) \left[ \frac{2(X_i - PP)}{FWHM} \right]^2} + \frac{(1 - PG)}{1 + \left[ \frac{2(X_i - PP)}{FWHM} \right]^2} \right\} \quad (5)$$

- **Asymmetric Gaussian-Lorentzian:**

$$B(X_i, Q) = H \left\{ PG \cdot e^{-\ln(2) \left[ \frac{2(X_i - PP)}{FWHM} \right]^2} + \frac{(1 - PG)}{1 + \left[ \frac{2(X_i - PP)}{FWHM} \right]^2} + Tail \right\} \quad (6)$$

where:

$$Tail = TS \left\{ 1 - e^{\left[ -\ln(2) \left( \frac{2(X_i - PP)}{FWHM} \right)^2 \right]} \right\} \left\{ e^{\left[ \left( \frac{-6.9}{TL} \right) \left( \frac{2(X_i - PP)}{FWHM} \right) \right]} \right\}$$

and:

- $B(X_i, Q)$  functional value at energy point  $X_i$ ,
- $X_i$  binding energy value for data point  $i$ ,
- $PP$  binding energy of the peak's center,
- $H$  height of the peak at its center,

## A: Algorithms

FWHM	full width at half maximum of the peak,
PG	percent Gaussian (where 0 is 0% and 1.0 is 100%),
TL	tail length in half width at half maximum of the peak,
TS	tail scale factor.

Both the Gaussian and Gaussian-Lorentzian formulas should sufficiently define these functions, but the Asymmetric Gaussian-Lorentzian formula requires further clarification.

### **Asymmetric Gaussian-Lorentzian Formula**

The Asymmetric Gaussian-Lorentzian formula is a combination of the regular Gaussian-Lorentzian formula and an exponential Tail formula.

The exponential Tail formula is applied only to the higher binding energy side of the peak, thereby giving the peak an asymmetric shape. It is the product of an exponential function and a Gaussian peak shape. A pure Gaussian shape is used to determine the tail function, and a Gaussian-Lorentzian combination determines the shape of the symmetric portion of the peak.

The shape of the exponential tail is determined by the Tail Length parameter. Tail Scale, a scaling parameter, is then applied to the tail to properly size the tail to the symmetric portion of the curve.

The area calculation of the Asymmetric Gaussian-Lorentzian peak must be determined numerically. The integral defining the area under the exponential tail cannot be solved analytically. Again, the symmetric portion of the peak is a standard Gaussian-Lorentzian peak. The area under this portion can be determined by integrating (analytically) the Gaussian-Lorentzian formula and evaluating this integral. The tail curve produced by a given tail length can be calculated over the window in which the tail is significant, then integrated numerically. In this case, a summation technique is used. The terms used are the following:

P	parameter set (union of parameter sets Q, each of which define a single band or peak shape) used to define F(X,Y),
m	number of parameters in the parameter set P,
$\partial Y_i / \partial P_j$	partial derivative of F(X,P) with respect to parameter $P_j$ evaluated at $X_i$ ,
$(X_i, Y_i)$	set of experimental data points $Y_i$ over the energy steps $X_i$ ,
n	number of data points in the set,
$F(X, P)$	function (defined in terms of the parameter set P) that will be fit to the $(X, Y)$ data set,
$\chi^2$	$\frac{1}{n - m} \sum_{i=1}^n W_i [F(X_i, P) - Y_i]^2 ,$
$W_i$	weighting factor (defined as $1/Y_i$ ).

This routine obtains a weighted-least-squares fit of the function  $F(X_i, P_j)$  to the data values  $(X_i, Y_i)$  by means of stepwise Gaussian-Newton iterations of parameter  $P_j$ . Within each iteration, parameters are selected for modification in a stepwise manner.

## **A: Algorithms**

The parameter selected at a given step is the one that, differentially, makes the greatest reduction in the error sum of squares.

If necessary to avoid matrix singularity problems, only a subset of the parameters may be modified during a given iteration. In addition, parameters whose modification in a given iteration would lead to violations of the range defined for it are not modified. In effect, the iteration is performed “on the boundary” when it appears that the best fit occurs outside the parameter range.

Beginning with an initial set of parameter estimates for the parameter set, the program minimizes the  $\chi^2$  by means of stepwise Gaussian-Newton iterations. Convergence is reached when the relative change is less than 0.001 for two iterations.

### **Parameter Locking**

Position, FWHM, and area ratio locking introduce additional constraints into the optimization process and may produce a fit that is not as optimal as would be achieved in an unconstrained process.

When locking is present, all parameters that can be varied are varied within their boundary constraints. Due to the complex interaction between the various peak parameters and peak area, convergence of the fit with area locking may be slow and may not result in an optimal fit.

*NOTE: If the limits for the parameters are tight, it is possible for all parameters to be disregarded for boundary constraints. Generally, either tight limits or area ratio locking should be used, but not both.*

*At least some of the parameters must have fairly loose limits defined. If, however, the case arises where all parameters are disregarded, the routine attempts to find the parameter that when adjusted will produce the closest match to the given area ratio and reports the result to the operator.*

### **Convergence to a Local Minimum**

MultiPak’s Curve Fit routine is not guaranteed to find the absolute minimum least-squares solution. The algorithm “searches” the least-squares solution space for a minimum, but it is possible that this search may converge to a local minimum rather than the absolute minimum desired.

*NOTE: The performance of the Curve Fit algorithm is generally good. Do not spend time manually trying to produce a “perfect” fit. Let the computer perform the optimization unless poor convergence is encountered.*

If the routine *does* appear to be converging to a local minimum, the following steps can be taken:

1. Minimize the number of parameters used by selecting a simpler peak shape or defining fewer bands to define the synthetic peak shape. For example, a Gaussian peak shape use only three parameters whereas an Asymmetric

#### A: Algorithms

- shape uses six parameters , and too many peaks can yield an overly “relaxed” fit.
2. Select good initial band parameter values to increase the probability of optimal convergence. If an unsatisfactory fit is obtained, choose a new set of initial parameters “on the other side” of the solution sought; that is, if the fit produced a synthetic curve generally below the actual data, change the parameters to values above the data and press Fit again.

## Differentiation

The differentiation routine is used as a means of suppressing the background in cases in which the peak-to-background ratio is small. In PHI systems, differentiation is accomplished using the Savitzky-Golay convolution algorithm.

The concept of convolution is an expanded calculation of a moving average, in which a convolution function involving an odd number of data points is moved along the data curve. The data point being modified is at the center of the window. The new data value is the resultant when the values in the window are multiplied by the corresponding convolution coefficients (Table A-1). The coefficients are derived by the least squares method.

*NOTE: In general, the fewer points selected for the Differentiation routine, the sharper the differentiated peak shape and the greater the resultant noise. The larger the number of points specified, the broader the differentiated peak shape and the lower the resultant noise.*

*Usually, a number between 5 and 13 will provide good peak definition and a reasonable noise level.*

For example, in a 5-point differentiation, the third data point is the center point. Two data points before and two points after the center point will be used in determining the weighted average of the center point. Each data point value will be multiplied by its corresponding convolution coefficient from Table A-1. These results are then summed and divided by the appropriate normalizing factor. When the calculation is complete, the 5-point “window” will be advanced by one and the process repeated. The mathematical description of this process is:

$$Y_j^* = \frac{\sum_{i=-m}^{i=m} C_i Y_j + 1}{N} \quad (7)$$

where:

- |         |   |
|---------|---|
| j       | running index of the ordinate data in the original data table,            |
| $Y_j$   | original data point,  |
| $Y_j^*$ | recalculated (differentiated) data point,                                 |
| m       | $(2n - 1)/2$ , where n is the number of points specified by the operator, |
| N       | normalization factor (NORM value from Table A-1),                         |
| C       | convoluting integer from Table A-1.                                       |

## **A: Algorithms**

This computation assumes the data was acquired at 1 eV/step, but corrects the formula when the electron volts per step is different than 1, so that all data points available are used but the energy range for differentiation is still computed over an energy range of 1 eV/step and the number for differentiation (an odd number between 3 and 25) specified by the operator is used.

Because there are data points on only one side of each endpoint, the differentiation process changes. Only three points are used to differentiate an endpoint and its neighboring point, even if a higher number is specified. To calculate the differentiation for the endpoint, the neighboring point, the endpoint, and a duplicate of the endpoint are used. For the neighboring point calculation, the endpoint, the neighboring point, and the third point are used. For each subsequent data point, the number of points used in the differentiation routine is increased by two until the number specified for the routine by the operator is reached.

## A: Algorithms

*Table A-1. Convoluting Coefficients for Differentiation.*

POINTS	25	23	21	19	17	15	13	11	9	7	5	3
-12	-12											
-11	-11	-11										
-10	-10	-10	-10									
-09	-9	-9	-9	-9								
-08	-8	-8	-8	-8	-8							
-07	-7	-7	-7	-7	-7	-7						
-06	-6	-6	-6	-6	-6	-6	-6					
-05	-5	-5	-5	-5	-5	-5	-5	-5				
-04	-4	-4	-4	-4	-4	-4	-4	-4	-4			
-03	-3	-3	-3	-3	-3	-3	-3	-3	-3	-3		
-02	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	-2	
-01	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
00	0	0	0	0	0	0	0	0	0	0	0	0
01	1	1	1	1	1	1	1	1	1	1	1	1
02	2	2	2	2	2	2	2	2	2	2	2	2
03	3	3	3	3	3	3	3	3	3	3	3	3
04	4	4	4	4	4	4	4	4	4			
05	5	5	5	5	5	5	5	5	5			
06	6	6	6	6	6	6	6	6				
07	7	7	7	7	7	7						
08	8	8	8	8	8							
09	9	9	9	9								
10	10	10	10									
11	11	11										
12	12											
NORM	<b>1300</b>	<b>1012</b>	<b>770</b>	<b>570</b>	<b>408</b>	<b>280</b>	<b>182</b>	<b>110</b>	<b>60</b>	<b>28</b>	<b>10</b>	<b>2</b>

## **FWHM/Area...**

In MultiPak, the FWHM (full width at half maximum) of a peak is determined in the following way.

1. The background is calculated by the specified background algorithm and subtracted from the data.
2. The first occurrence of a counts value less than or equal to half of the peak counts is found on both sides of the peak energy.
3. The exact energy corresponding to the half maximum is determined by interpolating between the surrounding energies.
4. The full width is set to the difference between the energies of these occurrences.
5. The noise reported is calculated as the root mean squared difference between the data and a second-order polynomial fit to the data around the right (low BE or high KE) analysis region cursor:

$$\sqrt{\frac{\sum_{i=1}^n (y_i - \bar{y}_i)^2}{(n-1)}} \quad (8)$$

where

- n      total number of points around the right (low BE or high KE) region cursor (n = 5 in MultiPak™ 6.0),  
y<sub>i</sub>    actual data curve,  
 $\bar{y}_i$     value of a second-order polynomial fit.

6. The Peak-To-Noise (P/N) is calculated by dividing Peak Height by Background Noise.
7. ISO Peak is calculated based on ISO 15472.

## **Linear Least Squares Fit**

The LLS (linear least squares) routine is presented in detail in an article in *Surface Interface Analysis* (15:516, 1990) by Physical Electronics scientist David G. Watson.

## Peak Area

Peak area is determined by defining a background between the two analysis region boundaries, then calculating the area under the curve and above the background.

## Peak Height

Peak height is determined by defining a background between the two analysis region boundaries, then calculating the maximum y value between the curve and the background.

## Peak to Peak

The peak-to-peak measurement is a calculation of the difference between the lowest y point on the curve and the highest y point on the curve between the two analysis region boundaries. This “Intensity Type” selection is available for AES data only. Differentiation should be performed prior to this calculation.

*NOTE: AES data that will have atomic concentrations calculated using MultiPak should have a 5-point differentiation applied **only**. This matches the data use to create the sensitivity factors used in the calculation.*

## Satellite Subtract

This ESCA Spectrum window function is used to remove x-ray source satellite lines from measured spectra. The routine is intended for data obtained with non-monochromatic Al or Mg x-ray source.

The satellites are subtracted as follows:

$$D(n) = D(n) - f_3 D\left(\frac{n - dE_3}{s}\right) - f_4 D\left(\frac{n - dE_4}{s}\right) - f_5 D\left(\frac{n - dE_5}{s}\right) - \\ f_6 D\left(\frac{n - dE_6}{s}\right) - f_B D\left(\frac{n - dE_B}{s}\right) \quad (9)$$

where:

$f_3, f_4, f_5, f_6$ , and  $f_B$  are relative height factors for each satellite;  
 $dE_3, dE_4, dE_5, dE_6$ , and  $dE_B$  are energy displacements for each satellite,  
 $s$  is the energy step size used for the acquisition,  
 $D(n)$  is the intensity at the  $n$ th data point, which is associated with an energy equal to the (starting energy) – ( $n \times s$ ).

#### **A: Algorithms**

The relative height factors and energy displacements are given in Table A-2 for magnesium and Table A-3 for aluminum.

If the energy displacement for a satellite is not an integral step size, the intensity at that displacement is determined by linear interpolation of the intensities of the two immediate surrounding data points.

If the energy displacement falls outside the energy window over which data was acquired, its intensity is set to that of the first data point after it has had all its satellites subtracted. In this way, the highest binding energy intensities (those within  $E_B$ , which is 48.5 eV for Mg and 69.7 eV for Al) will be affected by the “satellites” associated with the highest-binding-energy data point’s intensity.

*Table A-2. Mg-Anode Relative Height Factors and Energy Displacements.*

Variable	3	4	5	6	B
f (%)	8.0	4.1	0.55	0.45	0.50
dE (eV)	8.4	10.2	17.5	20.0	48.5

*Table A-3. Al-Anode Relative Height Factors and Energy Displacements.*

Variable	3	4	5	6	B
f (%)	6.4	3.2	0.40	0.30	0.55
dE (eV)	9.8	11.8	20.1	23.4	69.7

## Sensitivity Factors

The sensitivity factors contained in the Periodic Table databases for AES and ESCA are used in atomic concentration calculations.

### ***AES Periodic Table Sensitivity Factors***

MultiPak is capable to calculate an atomic concentration from the spectrum with CMA and with SCA analyzer. In the CMA analyzer, any energy resolution is available as far as it is not HR mode. On the other hand, in the SCA analyzer the energy resolution shall be 0.6%, 0.4%, 0.1%, and 0.1%. Their sensitivity factor corresponds to the peak-to-peak intensity of spectrum applied the differential with 4eV range, which corresponds 5 points differential in 1eV step acquisition. Sensitivity factors for both CMA analyzer and SCA analyzer in 0.6% energy resolution are included originally database file in MultiPak. When calculating an atomic concentration with spectrum acquired with CMA analyzer or SCA analyzer in 0.6% energy resolution mode, it is directly calculated with peak-to-peak intensity and sensitivity factor. When calculating an atomic concentration with spectrum acquired with SCA analyzer in 0.1% energy resolution mode, it is calculated with peak-to-peak intensity which is differentiated to the broadening spectrum corresponded to 0.6% and sensitivity factor. See Periodic Table in section 1 regarding sensitivity factors in each database file.

Note: Set energy cursors wider, taking account of the broadening process for spectrum, when calculating an atomic concentration in acquiring with SCA analyzer in 0.1% energy resolution mode. Adjust the range between energy cursors to be more than 6eV for 1000eV peak and more than 12eV for 2000eV peak, since spectrum gets to broaden about 0.6% of peak energy.

Note: The atomic concentration in acquiring with SCA analyzer in less than 0.1% energy resolution mode is not guaranteed.

Note: The sensitivity factor at arbitrary beam voltage is calculated from the database using linear interpolation..

Elemental relative sensitivity factors and Average matrix relative sensitivity factors.

Two types of relative sensitivity factors (RSF) are available in MultiPak. One is elemental relative sensitivity factors (ERSF), which are available for all versions. The other is average matrix relative sensitivity factors (AMRSF), which are available for version 9.2 or later. ERSFs are selected at the original installation

## A: Algorithms

for compatibility with prior versions. To switch the RSF from ERSF/AMRSF to AMRSF/ERSF, refer to Section 3 "Periodic Table".

The ERSFs were calculated on peak-to-peak data for three beam voltages (3, 5, and 10 keV).

The AMRSFs for 3, 5 and 10 kV are calculated from ERSFs for corresponding beam voltage and the matrix effect corrections based on the ISO18118:2004\*. The AMRSFs for 15, 20, 25 and 30 kV are calculated from AMRSFs at 10 kV and energy dependent calculation of ionization cross section and backscattering correction. Though the backscattering correction in ISO18118:2004 is limited to 10 kV, these calculations are extrapolated up to 30 kV in the literature on the consideration of the validity.

These values (ERSFs and AMRSFs) are valid only for data that have had a 5-point derivative applied to them. (The sensitivity factors can be made valid for a different number of differentiation points by editing this value in the Periodic Table's Transition dialog box.)

*NOTE: If the beam voltage doesn't match the database, a linear interpolation is done to find the sensitivity factor.*

*NOTE: When the RSFs are switched from ERSFs to AMRSFs, quantification results are generally changed. If you do not like the change of quantification, please continue to apply ERSF.*

### **RSF correction for the 4700TFA and VersaProbe II**

Atomic concentration calculations for AES data measured with 4700TFA or VersaProbe II uses corrected RSFs for those systems. Correction is made as follows:

$$S_{SCA} = S_{DB} / (c_0 + c_1E + c_2E^2 + c_3E^3)$$

Where:

$S_{DB}$  Relative sensitivity factor in the database

$S_{SCA}$  Corrected relative sensitivity factor

E Kinetic energy of the Auger electron (in kV)

$c_n$  Coefficients for polynomial function

$$c_0 = 0.4900$$

$$c_1 = 1.3465$$

---

\* ISO18118:2004 Surface chemical analysis – Auger electron spectroscopy and X-ray photoelectron spectroscopy – Guide to the use of experimentally determined relative sensitivity factors for the quantitative analysis of homogeneous materials

## **A: Algorithms**

$$c_2 = -1.2800$$

$$c_3 = 0.3548$$

*NOTE: Use 0.6% energy resolution data for AC calculations.*

### **ESCA Periodic Table Sensitivity Factors**

The sensitivity factors contained in the ESCA Periodic Table database were calculated for area and height data and assume:

- Analyzer transmission independent of energy,
- Source angle of 54.7 deg (the “magic angle” for which no asymmetry correction is needed).

Since different instruments have different transmissions, the ESCA sensitivity factors need to be adjusted to account for non-unity transmission of individual analyzers. They also need to be adjusted if the angle between the x-ray source and the analyzer (“source angle”) is different than 54.7 deg.

### **Transmission Function Correction**

MultiPak uses the coefficients entered by the operator using the Intensity Calibration function (Tools menu).

The a and b coefficients are generally different for each magnification and lens aperture setting of the OMNI Focus lenses. In fact, these systems have 15 possible combinations of magnification and aperture. The Quantum 2000, Quantera and VersaProbe have two lens modes, normal and narrow acceptance angle. The transmission function correction algorithm makes it possible to quantify spectra with mixed pass energies in a single multiplex, but it is good practice to take the data at a single pass energy.

## **A: Algorithms**

The analyzer transmission function describes the energy dependence (and pass energy dependence) of photoelectron peak areas. In functional model method, this energy dependence is a property of the spherical capacitance analyzer (SCA) and has been found to be well approximated by:

$$\frac{A}{E_p} = \left( \frac{a^2}{a^2 + R^2} \right)^b \quad (10)$$

where:

- |       |   |
|-------|---|
| $A$   | peak area,  |
| $E_p$ | pass energy,  |
| $R$   | retard ratio, given by $\frac{E_i}{E_p}$ , where $E_i$ is the initial kinetic energy. |

Measuring the transmission function and determining the correction coefficients is done by collecting data from three spectral regions on a sputter cleaned the sample at multiple pass energies. The values of  $a$  and  $b$  are determined by a least-squares fit of the copper data to the formula shown in equation 10.

### ***Source Angle Correction***

The correction factors can be computed to account for the angle between the x-ray source and the analyzer at which the data was acquired. When an atomic concentration calculation is performed by MultiPak, the sensitivity factors for 54.7 deg, which are contained in MultiPak's ESCA Periodic Table database and are listed in Appendix B, are multiplied by this correction factor to provide a source angle correction.

## A: Algorithms

For unpolarized x-ray radiation and randomly oriented atoms, the angular distribution factor ( $\Phi$ ) is given by:

$$\Phi = [1 - .25\beta(3\cos^2\theta - 1)] / 4\pi \quad (11)$$

where:

$\beta$       asymmetry parameter,  
 $\theta$       angle between the incident x-ray radiation and the observed photoelectron as it leaves the atom.

The angular distribution factor, therefore, expresses the geometric asymmetry in the photoabsorption and resulting photoemission process. The angular distribution factor for core orbitals is, therefore, independent of molecular structure.\*

The  $\beta$ 's have been calculated by Reilman et al.(Figure A-1) and are included in MultiPak's ESCA database. MultiPak uses the value of  $\theta$  (included in the header of every PHI data file) and the tabulated  $\beta$ 's in the above equation when calculating atomic concentration, but this is automatic and completely transparent to the user.

*Note: Although it is not necessary, MultiPak divides the calculated asymmetry value ( $\Phi$ ) for each peak by the asymmetry value of an "s" orbital before applying the asymmetry correction. This additional step has no impact on quantitative results but does impact reported values for the corrected sensitivity factors used in a specific calculation.*

The asymmetry parameter can have values between -1 and 2. Figure A-1 shows the angular distribution factor resulting from several values of  $\beta$ . For  $\beta = 0$ , the angular distribution is isotropic. Note that the observed ratio of two photoelectron peaks can change by as much as 230% in going from 45 deg to 90 deg between the x-ray trajectory and detected photoemission. Because values of  $\beta$  usually fall between 0.8 and 2.0, changes in relative photoemission intensities of 50% are likely for different ESCA instrument geometries.

The difference in asymmetry parameter for Al K $\alpha$  –x-ray vs Mg K $\alpha$  –x –ray is small enough that. MultiPak uses the asymmetry parameter for Al K $\alpha$  – x-rays for both Al and Mg XPS data.

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\* J.C. Tully, R.S. Berry, and B.J. Dalton, *Physical Review*, **176**:95, (1968); and J. Cooper and R.N. Zare, *Journal of Chemical Physics*, **48**:942, (1968).

### A: Algorithms

This change in relative photoemission intensities for different instrument geometries is one reason for the difficulties reported in comparing ESCA data between laboratories.<sup>†</sup>

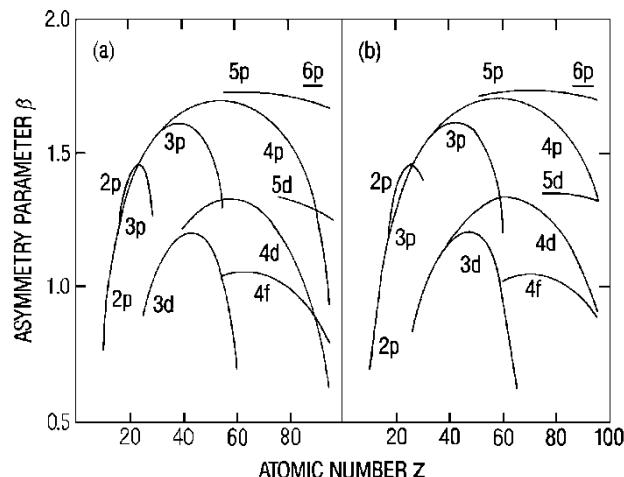


Figure A-1.

Asymmetry parameter according to Reilman et al.

---

<sup>†</sup> M.P. Seah, in *Practical Surface Analysis*, D. Briggs and M.P. Seah, eds., New York: J. Wiley and Sons, pp. 200–201, (1983).

## Smooth

Smoothing reduces the noise evident in a spectrum, improves the visual presentation of the data and facilitates enhanced data interpretation. Smoothing is accomplished in MultiPak by either the Savitzky-Golay convolution algorithm<sup>14</sup> or the Binomial algorithm.

### **Savitzky-Golay Convolution Algorithm**

The concept of convolution is an expanded calculation of a moving average. Referring to Table A-4, a 5-point smooth is shown. The C's represent any set of convoluting integers. There is an associated normalizing or scaling factor. The procedure is to multiply  $C_{-2}$  by the number opposite it,  $C_{-1}$  by its number, etc., sum the results, and divide by the normalizing factor, if appropriate. The result is the desired function evaluated at the point indicated by  $C_0$ .

For the next point, the set of convoluting integers is moved down and the process is repeated. The mathematical description of this process is:

$$Y_j^* = \frac{\sum_{i=-m}^{i=m} C_i Y_j + 1}{N} \quad (12)$$

where:

$j$	running index of the ordinate data in the original data table,
$Y_j$	original data point,
$Y_j^*$	recalculated (smoothed) data point,
$m$	$(2n - 1)/2$ , where $n$ is the number of points specified by the operator,
$N$	normalization factor (NORM value from Table A-5),
$C$	convoluting integer from Table A-4.

---

<sup>14</sup> Abraham Savitzky and Marcel J.E. Golay, "Smoothing and Differentiation of Data by Simplified Least Squares Procedures," *Analytical Chemistry*, **36**:8, (July 1964).

## A: Algorithms

Table A-4. Savitzky-Golay Smoothing Operation.

Abscissa	Convolution Integers, $C_i$		Tabular Data
1800.0			705
1799.8			712
1799.6			717
1799.4			718
1799.2			721
1799.0			722
1798.8	$x_0^{-2}$	$C_{-2}$	725
1798.6	$x_0^{-1}$	$C_{-1}$	730
1798.4	$x_0^0$	$C_0$	735
1798.2	$x_0^{+1}$	$C_1$	736
1798.0	$x_0^{+2}$	$C_2$	741
1797.8			746
1797.6			750

Because there are data points on only one side of each endpoint, the smooth process changes. Only three points are used to smooth an endpoint and its neighboring point, even if a higher number is specified. To calculate the smooth for the endpoint, the neighboring point, the endpoint, and a duplicate of the endpoint are used. For the neighboring point calculation, the endpoint, the neighboring point, and the third point are used. For each subsequent data point, the number of points used in the smooth is increased by two until the number specified for the routine by the operator is reached.

### Binomial Algorithm

The Binomial algorithm used in MultiPak is presented in detail in an article in *Review of Scientific Instrumentation* (**54**:8, pp. 1034, 1983) by Marchand and Marmet. Generally, this is a weighted average. While it is better at removing periodic noise, some details of the peak shape may be lost with this method.

### A: Algorithms

*Table A-5. Convoluting Coefficients and Normalization Factors for Smoothing.*

POINTS	25	23	21	19	17	15	13	11	9	7	5	3
-12	-253											
-11	-138	-42										
-10	-33	-21	-171									
-09	62	-2	-76	-136								
-08	147	15	9	-51	-21							
-07	222	30	84	24	-6	-78						
-06	287	43	149	89	7	-13	-11					
-05	342	54	204	144	18	42	0	-36				
-04	387	63	249	189	27	87	9	9	-21			
-03	422	70	284	224	34	122	16	44	14	-2		
-02	447	75	309	249	39	147	21	69	39	3	-3	
-01	462	78	324	264	42	162	24	84	54	6	12	1
00	467	79	329	269	43	167	25	89	59	7	17	2
01	462	78	324	264	42	162	24	84	54	6	12	1
02	447	75	309	249	39	147	21	69	39	3	-3	
03	422	70	284	224	34	122	16	44	14	-2		
04	387	63	249	189	27	87	9	9	-21			
05	342	54	204	144	18	42	0	-36				
06	287	43	149	89	7	-13	-11					
07	222	30	84	24	-6	-78						
08	147	15	9	-51	-21							
09	62	-2	-76	-136								
10	-33	-21	-171									
11	-138	-42										
12	-253											
NORM	<b>5175</b>	<b>805</b>	<b>3059</b>	<b>2261</b>	<b>323</b>	<b>1105</b>	<b>143</b>	<b>429</b>	<b>231</b>	<b>21</b>	<b>35</b>	<b>4</b>

## Target Factor Analysis

The following subsections describe the algorithms used in the TFA routine.\*

### ***Principal Component Analysis (PCA) Using Singular Value Decomposition***

$D = U \cdot S \cdot V'$ = $R \cdot C$	Singular value decomposition of spectral data matrix.
U	Orthonormal eigenvector that spans the row space.
V	Orthonormal eigenvector that spans the column space.
S	Diagonal singular value matrix with positive diagonal singular values in decreasing order.
$R = U \cdot S$	Abstract component spectra in columns.
$C = V'$	Abstract component concentration profiles in rows.
$\Lambda = S^2$	Diagonal eigenvalue matrix with positive diagonal eigenvalues ( $\lambda$ ) in decreasing order. Each eigenvalue represents a portion of the total variance in the spectral data matrix.
$\bar{D} = \bar{R} \cdot \bar{C}$	PCA-reconstructed (PCA-smoothed) spectra that uses only principal components.

### ***Log( $\lambda$ ) function***

The eigenvalues of principal components are significantly different from those of error components. The magnitude of all error eigenvalues is approximately the same if the experimental errors are *randomly and uniformly distributed* over the whole matrix of spectral data.

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\* Much of this work drew from the work of E.R. Malinowski, *Factor Analysis in Chemistry*, John Wiley & Sons, (1991).

## A: Algorithms

### Real Error or Residual Standard Deviation

$$RE = RSD = \left( \frac{\sum_{j=n+1}^c \lambda_j}{r(c-n)} \right)^{1/2} \quad (13)$$

$r$  is either the number of rows in the data matrix  $\mathbf{D}$  or the number of columns in the data matrix  $\mathbf{D}$ , whichever is larger.  $c$  is either the number of columns in the data matrix  $\mathbf{D}$  or the number of rows in the data matrix  $\mathbf{D}$ , whichever is smaller.  $n$  is the number of principal components selected.

RE measures the difference between pure and raw data. Once the correct number of principal components is used for the reconstruction, the RE should be approximately equal to the estimated *experimental error* of the data.

### Imbedded Error

$$IE = RE \sqrt{\frac{n}{c}} \quad (14)$$

IE measures the difference between PCA-reconstructed and pure data. Once the correct number of principal components is used for the reconstruction, the IE(n) should reach a minimum, if the experimental error is *randomly and uniformly distributed* over the whole matrix of spectral data.

### Indicator Function

$$IND = \frac{RE}{(c-n)^2} \quad (15)$$

Similar to IE, once the correct number of principal components is used for the reconstruction, the IND(n) should reach a minimum, even when IE(n) exhibits no minimum.

### Percent Variance

$$\%Var = 100 \times \frac{\lambda_n}{\sum_{j=1}^c \lambda_j} \quad (16)$$

Principle components should have larger variances than error components. However, classifying the variance as large or small could be a problem.

### Cumulative Percent Variance

$$sum(\%Var) = 100 \times \frac{\sum_{j=1}^n \lambda_j}{\sum_{j=1}^c \lambda_j} \quad (17)$$

## A: Algorithms

This value measures the total percentage variance that is accounted for by the principal components. The cumulative percent variance criterion is to accept the set of components of the largest eigenvalues as principal components so that a specified portion of the total variance is accounted for by the principal components. However, an arbitrary specification such as 90%, 95%, or 99% variance is not reliable without a knowledge of the true variance and the error in the data.

### **Significance of Eigenvalues**

$$SOE = \sqrt{\frac{\lambda_n}{\sum_{j=n+1}^c \lambda_j}} \quad (18)$$

An eigenvalue belongs to the primary group if SOE is greater than 1. MultiPak uses the SOE value to determine how many eigenvalues belong to the primary group. However, the arbitrary value of 1 is not reliable without knowledge of the true variance and the error in the data.

### **F-test on Reduced Eigenvalues**

Reduced eigenvalues:

$$REV_n = \frac{\lambda_n}{(r-n+1)(c-n+1)} \quad (19)$$

Weighted average of the pool of the reduced error eigenvalues:

$$REV_{pool}^0 = \frac{\sum_{j=n+1}^c \lambda_j}{\sum_{j=n+1}^c (r-j+1)(c-j+1)} \quad (20)$$

F-test on reduced eigenvalues (Any eigenvalue  $\lambda_n$  that is not an error eigenvalue will have  $REV_n$  value significantly larger than  $REV_{pool}^0$  .):

### **F-test on Reduced Eigenvalues**

$$F(1, c-n) = \frac{REV_n}{REV_{pool}^0} \quad (21)$$

A small percent significance level (%SL) at which the null hypothesis “ $REV_n$  is equal to  $REV_{pool}^0$  ” can be rejected implies a very significant rejection, in turn implying high confidence in the hypothesis “ $REV_n$  is larger than  $REV_{pool}^0$  ” (one-tailed F-test).

## **A: Algorithms**

The determination of the minimum number of active components starts from the lowest eigenvalue, so that  $n$  is changed from  $c-1$  for the lowest eigenvalue to 1 for the highest eigenvalue. If the %SL for an eigenvalue is smaller than the reference level (5% or 10%), the components represented by this eigenvalue and other eigenvalues that are greater than this eigenvalue should be considered as principal components.

### **Testing of a Target Spectrum $x_i$**

$$t_i = (\bar{R} \cdot \bar{R})^{-1} \cdot \bar{R} \cdot x_i \quad (22)$$

where:

$$\hat{x}_i = \bar{R} \cdot t_i \quad \text{Predicted spectrum vector}$$

$$T = [t_1, t_2, \dots, t_n] \quad \text{Complete transformation matrix}$$

$$R = \bar{R} \cdot T \quad \text{Predicted component spectra in columns}$$

$$C = T^{-1} \cdot \bar{C} \quad \text{Predicted component concentration vector in rows}$$

If not all the data points of  $x$  are known, then only those rows of  $\bar{R}$  in  $t_i$  expression that correspond to the known data points in  $x$  are used for testing (free-float target-testing of a target spectrum). A complete spectrum is always produced even when an incomplete target spectrum is used for the testing.

### **Testing of a Target Concentration Profile**

This is done in a fashion similar to that of target spectra testing.

## Thickness...

When the film thickness of a uniform thin film on a smooth surface is less than the escape depth of photoelectrons used for ESCA measurements (typically, <50Å), photoelectrons from both the film and the substrate are observed, and the relative intensities of the film and substrate peaks can give a measure of the film thickness at a particular location.

Assuming the binding energies of the film and substrate peaks are very similar, the thickness ( $d$  in Å) can be calculated from ESCA spectra using the equation:

$$d = \lambda \sin \theta \ln \left[ \left( \frac{I_F + I_F * OV}{I_S - I_F * OV} \right) * a + 1 \right]^{15,16,17,18} \quad (23)$$

where

- $I_F$  = Intensity of the peak corresponding to the film,
- $I_S$  = Intensity of the peak corresponding to the substrate,
- $\lambda$  = Inelastic mean free path or attenuation length of electrons in the film,
- $\theta$  = Take-off angle above the plane of the sample for detection of electrons,
- $OV$  = Correction factor for a peak overlap between the film and substrate
- $a$  = Ratio of sensitivity factors for substrate and film.

If  $OV$  is taken to be 0, the equation becomes:

$$d = \lambda \sin \theta \ln \left[ \left( \frac{I_F}{I_S} \right) * a + 1 \right] \quad (24)$$

The following consistency checks are performed on each spectrum to flag possibly invalid data:

- The area of the region composed of the background and the lines between the region cursors must be greater than 0 and must not be greater than 10% of the total area between the outermost endpoints. §
- The areas of both the film and substrate peaks must be greater than 0, and the ratio of the film to substrate peak areas must be less than 20. ‡, §
- The value of the quantity  $I_S + a * I_F$  should be a constant from one spectrum to the next, so that no spectrum should have a value for this quantity that is

15 M.P. Seah in *Practical Surface Analysis, Vol. 1: Auger and X-ray Photoelectron Spectroscopy, 2<sup>nd</sup> Edition*, D. Briggs and M.P. Seah, eds., Wiley: Chichester. (1990).

16 C.S. Fadley in *Progress in Surface Science, Vol. 16*, S.G. Davidson, ed., Pergamon Press. (1984).

17 P.J. Cumpson and M.P. Seah, *Surface and Interface Analysis*, **25**, 430–446. (1997).

18 R. Linder, private communication. (August 1997).

## A: Algorithms

more than 5% above or below the average value for all spectra. This can flag Z-axis alignment errors.<sup>19</sup>

- The take-off angle  $\theta$ , which is taken from the data, should be the same for all spectra. If it is not the same for all spectra, the correct values will be used for the thickness calculation, but only one value will be output to the header of the text file.

## Topographical Correction

The Topographical Correction function corrects for the effects of specimen topography in line data by dividing the peak-height data by the corresponding background data:

$$\frac{N(E_p) - N(E_b)}{N(E_b)} \times N(E_b)_{\text{average}} \quad (25)$$

The expression is calculated at every point on the line. The background data values  $N(E_b)$  and peak values  $N(E_p) - N(E_b)$  are both stored during data acquisition. Multiplication by the average background value is included for normalization.

## Ultra Thin Film Analysis

### **Structure analysis:**

Structure analysis routine can estimate the layer order by measuring the change of peak intensity ratios of components between at two take-off angles (recommend 90 and less than 20 degrees TOA)<sup>20</sup>. This process can also estimate the layer thicknesses and compositions based on the estimated layer order. This process can be applied to the films where the thickness is similar to or less than effective attenuation length of the measured photoelectrons.

In this process, the order of film layers, film thickness and compositions are obtained based on some approximations and suppositions.

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19 R. Linder, private communication. (August 1997).

20 Simple method of depth profiling (stratifying) contamination layers, illustrated by studies on stainless steel: M. P. Seah, J. H. Qiu, P. J. Cumpson, and J. E. Castle, Surface and Interface Analysis, Vol. 21, Issue 6–7, pages 336–341, 1994

### **The estimation of layer order**

First, the peak intensity ratios of all components between the two take-off angles are measured. Then the layer order is estimated based on the magnitude correlations of peak intensity ratios.

The structure analysis function estimates the layer order by assuming each layer is composed of one component. If there are multiple layers on a substrate material, the photoelectron intensity of nth layer from the top layer is expressed as follows:

$$I_n = I^0 s_n \left[ 1 - \exp\left(-\frac{t_n}{\lambda_{n,n} \sin \theta}\right) \right] \prod_{i=1}^{n-1} \exp\left(-\frac{t_{n-i}}{\lambda_{n,n-i} \sin \theta}\right) \quad (26)$$

Here,  $I^0$  is the base intensity,  $s_n$  is relative sensitivity factor,  $t_n$  is the thickness of nth layer, and  $\lambda_{n,m}$  is the attenuation length in the mth layer where the electrons are generated in the nth layer. In this routine, attenuation length is calculated from equation (31), which is explained later.

The intensity of  $n+l$  th layer is expressed as follows:

$$I_{n+l} = I^0 s_{n+l} \left[ 1 - \exp\left(-\frac{t_{n+l}}{\lambda_{n+l,n+l} \sin \theta}\right) \right] \prod_{i=1}^{n+l-1} \exp\left(-\frac{t_i}{\lambda_{n+l,i} \sin \theta}\right) \quad (27)$$

When we divide intensity of  $n$  th layer by that of  $n+l$  th layer, the following equation is obtained.

$$\frac{I_n}{I_{n+l}} = \frac{s_n}{s_{n+l}} \cdot \frac{\left[ 1 - \exp\left(-\frac{t_n}{\lambda_{n,n} \sin \theta}\right) \right]}{\left[ 1 - \exp\left(-\frac{t_{n+l}}{\lambda_{n+l,n+l} \sin \theta}\right) \right]} \cdot \frac{\prod_{i=1}^{n-1} \exp\left(-\frac{t_i}{\lambda_{n,i} \sin \theta}\right)}{\prod_{i=1}^{n+l-1} \exp\left(-\frac{t_i}{\lambda_{n+l,i} \sin \theta}\right)} \quad (28)$$

If take-off angle is nearly 0 and the attenuation length of electron is independent of material, the following equation is obtained:

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$$\begin{aligned}
 \frac{I_n}{I_{n+l}} &\approx \frac{s_n}{s_{n+l}} \cdot \frac{\frac{t_n}{\lambda_{n,n}}}{\frac{t_{n+l}}{\lambda_{n+l,n+l}}} \cdot \frac{\exp\left(-\frac{t_{n-1} + \dots + t_1}{\lambda_{n,n} \sin \theta}\right)}{\exp\left(-\frac{t_{n+l-1} + \dots + t_1}{\lambda_{n+l,n+l} \sin \theta}\right)} \\
 &= \frac{s_n t_n \lambda_{n+l,n+l}}{s_{n+l} t_{n+l} \lambda_{n,n}} \cdot \exp\left(\frac{1}{\sin \theta} \left( \frac{(t_{n+l-1} + \dots + t_1)}{\lambda_{n+l,n+l}} - \frac{(t_{n-1} + \dots + t_1)}{\lambda_{n,n}} \right)\right) \quad (29)
 \end{aligned}$$

If equation (29) is differentiated with respect to take-off angle, the following equation is obtained:

$$\begin{aligned}
 \frac{\partial}{\partial \theta} \left( \frac{I_n}{I_{n+l}} \right) &\approx \frac{s_n t_n \lambda_{n+l,n+l}}{s_{n+l} t_{n+l} \lambda_{n,n}} \cdot \exp\left(\frac{1}{\sin \theta} \left( \frac{(t_{n+l-1} + \dots + t_1)}{\lambda_{n+l,n+l}} - \frac{(t_{n-1} + \dots + t_1)}{\lambda_{n,n}} \right)\right) \\
 &\quad \times \left( \frac{(t_{n+l-1} + \dots + t_1)}{\lambda_{n+l,n+l}} - \frac{(t_{n-1} + \dots + t_1)}{\lambda_{n,n}} \right) \left( \frac{-\cos \theta}{\sin^2 \theta} \right) \quad (30)
 \end{aligned}$$

The plus or minus of equation (30) is determined by the value of

$\left( \frac{(t_{n+l-1} + \dots + t_1)}{\lambda_{n+l,n+l}} - \frac{(t_{n-1} + \dots + t_1)}{\lambda_{n,n}} \right)$ . If  $\lambda_{n+l,n+l} \approx \lambda_{n,n}$ , the sign of equation (30)

becomes minus, because  $(t_{n+l-1} + \dots + t_1) > (t_{n-1} + \dots + t_1)$ . In the case of a two component system, the intensity ratio is obtained by dividing the intensity of component A by that of component B. If this ratio decreases near 0 degrees of take-off angle, component A locates above component B. However, it is difficult to measure the intensity change near 0 degrees take-off angle. Therefore, the intensity change is estimated by measuring the intensities at 90 and about 20 degrees take-off angle. Here,  $I_A^{\theta_H}$  is the intensity of component A at higher take-off angle, and  $I_A^{\theta_L}$  is that at lower take-off angle. Similarly, the intensities of component B at higher and lower take-off angles are  $I_B^{\theta_H}$  and  $I_B^{\theta_L}$  respectively.

Then the ratio,  $\frac{I_A^{\theta_L}}{I_B^{\theta_L}} / \frac{I_A^{\theta_H}}{I_B^{\theta_H}}$ , is calculated. If this ratio is larger than 1, component

A is located above component B. Based on this procedure, the positional relationship of all components can be estimated. If this ratio is close to 1, these components are assumed to be in the same layer.

(Note) This estimation process is based on the assumption that the attenuation lengths of electrons of all components are almost same as shown in equation (30). If the attenuation lengths are significantly different, the estimated structure may have error.

**The estimation of film thicknesses and compositions:**

A model for the film thickness and composition can be calculated using the relative positions of the layer structures and using intensity data from a large take-off angle using equation 26. The model is calculated assuming one element per layer. If prior information exists of multiple elements in a given layer, this information is included in the calculation. The calculation then iterates the model structure using the data from high and low take-off angle intensity data to produce the best fit to the data. It should be noted that changes in intensity produced by chemical shifts in peak positions as a function of depth are ignored in this calculation.

**The attenuation length used in the calculation:**

The attenuation length,  $\lambda$ , is expressed by the following equation<sup>21,22,23</sup>:

$$\lambda = K \cdot \alpha \cdot E^{\frac{3}{4}} \quad (31)$$

E is the kinetic energy (keV) of a photoelectron referenced to the Fermi edge,  $\alpha$  is the correction factor to the inelastic mean free path (TPP-2M)<sup>4</sup> which is a function of  $E^{\frac{3}{4}}$ . In this calculation,  $\alpha$  should be 2.1 for metals, 2.4 for inorganic compounds and 3.0 for organic compounds respectively. These values are derived from the mean values in the noted report<sup>2</sup>. Coefficient K is a value that depends on the take-off-angle of the energy analyzer and the elastic scattering of the photoelectrons

**Si-O-N depth profile:**

Si-O-N depth profile routine calculates the distribution of implanted N in SiO<sub>2</sub> thin film using the intensities of Si, O and N acquired at various take off angles.

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<sup>21</sup> Attenuation lengths of low-energy electrons in solids: C. J. Powell, Surface Science, Vol. 44, Issue 1, pages 29 – 46, (Jul. 1974)

<sup>22</sup> Calculations of Electron IMFPs IV. Evaluation of Calculated IMFPs and of the Predictive IMFP Formula TPP-2 for Electron Energies between 50 and 2000eV: S. Tanuma, C. J. Powell, D. R. Penn, Surface and Interface Analysis, Vol. 20, Issue 1, pages 77 – 89, (Jan. 1993)

<sup>23</sup> S. Tanuma, Electron Attenuation lengths, chapter 11 in Surface analysis by Auger and X-ray photoelectron spectroscopy, eds. D. Briggs and J. T. Grant: IM Publishing and Surface Spectra Limited, (2003), pages 259 – 294

## A: Algorithms

The implanted N is assumed to form  $\text{Si}_3\text{N}_4$  in the film. The N implanted  $\text{SiO}_2$  layer, (SiON layer), is divided into  $m$  equal bins. It is assumed that the summation of volumes of  $\text{SiO}_2$  and  $\text{Si}_3\text{N}_4$  is 1 in each bin. By changing the volume ratio between  $\text{SiO}_2$  and  $\text{Si}_3\text{N}_4$  in each bin, the signal intensity at each take-off angle is calculated. Then, the best fit distribution is obtained by finding the smallest residual error between acquisition data and calculated data using a least-squares method. Data at take-off angles from 20 to 90 degrees are recommended for use with the Si-O-N function. Below 20 degrees surface scattering and other effects become significant and are difficult to model.

### ***The estimation of film thickness:***

First the thickness of  $\text{SiO}_2$  layer is calculated. The thickness is calculated from the signal intensity ratio between the oxidized silicon and substrate silicon, using a method similar to the [Thickness] function described in this manual.

### ***The effective attenuation length (EAL) of the elements in each bin:***

To calculate signal intensities of elements, it is necessary to estimate EAL of N ( ${}^i\lambda_N^{\text{SiON}}$ ) , EAL of O ( ${}^i\lambda_O^{\text{SiON}}$ ) and EAL of Si ( ${}^i\lambda_{\text{Si}}^{\text{SiON}}$ ) in  $i$  th bin of SiON layer. These values are based on the volume ratio ( $x_i$ ) between  $\text{SiO}_2$  and  $\text{Si}_3\text{N}_4$  as follows:

$$\begin{aligned} {}^i\lambda_{\text{Si}}^{\text{SiON}} &= \frac{1}{\frac{x_i}{\lambda_{\text{Si}}^{\text{SiO2}}} + \frac{(1-x_i)}{\lambda_{\text{Si}}^{\text{Si3N4}}}} \\ {}^i\lambda_N^{\text{SiON}} &= \frac{1}{\frac{x_i}{\lambda_N^{\text{SiO2}}} + \frac{(1-x_i)}{\lambda_N^{\text{Si3N4}}}} \\ {}^i\lambda_O^{\text{SiON}} &= \frac{1}{\frac{x_i}{\lambda_O^{\text{SiO2}}} + \frac{(1-x_i)}{\lambda_O^{\text{Si3N4}}}} \end{aligned} \quad (32)$$

Here,  $\lambda_{\text{Si}}^{\text{SiO2}}$  is EAL of Si in SiON,  $\lambda_{\text{Si}}^{\text{Si3N4}}$  is EAL of Si in  $\text{Si}_3\text{N}_4$ ,  $\lambda_N^{\text{SiO2}}$  is EAL of N in  $\text{SiO}_2$ ,  $\lambda_N^{\text{Si3N4}}$  is EAL of N in  $\text{Si}_3\text{N}_4$ ,  $\lambda_O^{\text{SiO2}}$  is EAL of O in  $\text{SiO}_2$ , and  $\lambda_O^{\text{Si3N4}}$  is EAL of O in  $\text{Si}_3\text{N}_4$ .

## A: Algorithms

### **Signal intensities of elements:**

The numbers of atoms of Si, N, O ( ${}^iQ_{Si}$ ,  ${}^iQ_N$ ,  ${}^iQ_O$ ) in  $i$  th bin are expressed as follows:

$$\begin{aligned} {}^iQ_{Si} &= \phi_{Si}^{SiO_2} \cdot x_i + \phi_{Si}^{Si_3N_4} \cdot (1 - x_i) \\ {}^iQ_N &= \phi_N^{Si_3N_4} \cdot (1 - x_i) \\ {}^iQ_O &= \phi_O^{SiO_2} \cdot x_i \end{aligned} \quad (33)$$

Here,  $\phi_{Si}^{SiO_2}$  is the density of Si in  $SiO_2$ ,  $\phi_{Si}^{Si_3N_4}$  is that of Si in  $Si_3N_4$ ,  $\phi_N^{Si_3N_4}$  is that of N in  $Si_3N_4$ , and  $\phi_O^{SiO_2}$  is that of O in  $SiO_2$ . The signal intensities of elements ( $I_{Si}$ ,  $I_N$ ,  $I_O$ ) from the provided depth distribution is expressed as follows, when the thickness of each bin is  $d$ .

$$\begin{aligned} I_{Si} &= I^0 \alpha_{Si} \sum_{i=1}^N \left[ {}^iQ_{Si} \cdot \prod_{j=1}^{i-1} \exp\left(\frac{-d}{j \lambda_{Si}^{SiON} \sin \theta}\right) \left(1 - \exp\left(\frac{-d}{i \lambda_{Si}^{SiON} \sin \theta}\right)\right) \right] \\ I_N &= I^0 \alpha_N \sum_{i=1}^N \left[ {}^iQ_N \cdot \prod_{j=1}^{i-1} \exp\left(\frac{-d}{j \lambda_N^{SiON} \sin \theta}\right) \left(1 - \exp\left(\frac{-d}{i \lambda_N^{SiON} \sin \theta}\right)\right) \right] \\ I_O &= I^0 \alpha_O \sum_{i=1}^N \left[ {}^iQ_O \cdot \prod_{j=1}^{i-1} \exp\left(\frac{-d}{j \lambda_O^{SiON} \sin \theta}\right) \left(1 - \exp\left(\frac{-d}{i \lambda_O^{SiON} \sin \theta}\right)\right) \right] \\ I_{Sub} &= I^0 \alpha_{Si} \phi_{Si}^{SiO_2} \cdot \prod_{i=1}^N \exp\left(\frac{-d}{i \lambda_{Si}^{SiON} \sin \theta}\right) \end{aligned} \quad (34)$$

Here,  $I^0$  is base intensity, and relative atomic sensitivity factors of Si, N, O are  $\alpha_{Si}$ ,  $\alpha_N$ ,  $\alpha_O$ , respectively.  $I_{Sub}$  is signal intensity of Si substrate.

### **The depth distribution of $Si_3N_4$ :**

It is very difficult to unambiguously determine the distribution of an element in a thin film from ARXPS data alone<sup>24</sup>. This is because the signal intensity of an element in a material is reduced exponentially relative to the distance from surface. Therefore, some assumptions are necessary to determine the depth distribution of element. In this routine, the distribution of  $Si_3N_4$  is assumed to have a Gaussian distribution as described by the following equation:

<sup>24</sup> Distinguishability of N composition profiles in SiON films on Si by angle-resolved x-ray photoelectron spectroscopy, C. J. Powell, W. S. M. Welner and W. Smekal, Applied Physics Letters 89, 172101(2006).

## A: Algorithms

$$G(x) = h \cdot \exp\left(\frac{-(x-u)^2}{2\sigma^2}\right) \quad (35)$$

Here,  $h$  is the maximum value (the maximum volume ratio),  $u$  is the median value (the position which gives the maximum volume ratio), and  $\sigma$  is the standard deviation. In this routine, the user is requested to enter FWHM ( $w$ ). If the user does not enter FWHM, the default value 0.2[nm] will be entered. The relationship between FWHM and the standard deviation is expressed as follows:

$$\sigma = \frac{w}{2\sqrt{2\ln(2)}} \quad (36)$$

In this routine, based on the entered FWHM value, the signal intensities of the elements are calculated by changing the maximum value ( $h$ ) and the median value ( $u$ ). Then the best fit  $h$  and  $u$  are obtained by finding the smallest residual error between acquisition data and calculated data based on a least-squares method.

Then, the distributions of Si, N and O ( $G_{Si}, G_N, G_O$ ) is expressed as follows:

$$\begin{aligned} G_{Si}(x) &= \phi_{Si}^{Si3N4} \cdot G(x) + \phi_{Si}^{SiO2} \cdot (1 - G(x)) \\ G_N(x) &= \phi_N^{Si3N4} \cdot G(x) \\ G_O(x) &= \phi_O^{SiO2} \cdot (1 - G(x)) \end{aligned} \quad (37)$$

Therefore, the concentration distribution of N ( $G'_N$ ) is expressed as follows:

$$G'_N(x) = \frac{G_N(x)}{G_N(x) + G_O(x) + G_{Si}(x)} = \frac{\phi_N^{Si3N4} \cdot G(x)}{(\phi_N^{Si3N4} + \phi_{Si}^{Si3N4} - \phi_O^{SiO2} - \phi_{Si}^{SiO2}) \cdot G(x) + \phi_O^{SiO2} + \phi_{Si}^{SiO2}} \quad (38)$$

If the following parameters are introduced, the above equation is expressed as follows:

$$\begin{aligned} \xi_{Si3N4} &= \frac{\phi_N^{Si3N4} + \phi_{Si}^{Si3N4}}{\phi_N^{Si3N4}} \\ \xi_{SiO2} &= \frac{\phi_O^{SiO2} + \phi_{Si}^{SiO2}}{\phi_N^{Si3N4}} \\ G'_N(x) &= \frac{G(x)}{(\xi_{Si3N4} - \xi_{SiO2}) \cdot G(x) + \xi_{SiO2}} \end{aligned} \quad (39)$$

## A: Algorithms

Because the maximum volume ratio of N ( $h$ ) is the value at  $x = u$ , this value is expressed as follows:

$$G'_N(u) = \frac{G(u)}{(\xi_{Si3N4} - \xi_{SiO2}) \cdot G(u) + \xi_{SiO2}} = \frac{h}{(\xi_{Si3N4} - \xi_{SiO2}) \cdot h + \xi_{SiO2}}$$

$$h = \frac{\xi_{SiO2} G'_N(u)}{1 - (\xi_{Si3N4} - \xi_{SiO2})} \quad (40)$$

### **The calculation of dose amount of N:**

The dose of N (atoms / cm<sup>2</sup>) is the number of atoms of N ( $D_N$ ) at [1 cm x 1 cm x total film thickness of SiON]. Therefore,  $D_N$  is calculated as follows:

$$D_N = \int_0^{SiONthickness} G_N(x) dx \cdot \phi_N^{Si3N4} \quad (41)$$

## Appendix B: XPS Sensitivity Factors

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The sensitivity factors contained in MultiPak's ESCA database were calculated for both peak area and height data and assume an analyzer transmission that is independent of energy and an x-ray source angle of 54.7 deg. The database can be modified by the user, as described in Section 3, "Transition Dialog Box." For more information about the use of the ESCA sensitivity factors, refer to Appendix A, "Sensitivity Factors."

Element	Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡
			Area	Height	High	Low	High	Low			
Aluminum Al 13	Al2p	74	0.256	0.249	88	68	87	69	3	1	2
		119	0.312	0.230	133	113	132	114	2	1	2
Antimony Sb 51	Sb3d3	539	3.649	3.318	549	529	548	530	2	1	2
	Sb3d5	530	5.334	5.334	543	523	542	524	3	1	2
	Sb3p1	814	0.809	0.355	824	804	823	805	2	1	2
	Sb3p3	768	1.733	0.657	778	758	777	759	2	1	2
	Sb4d	34	1.405	1.208	48	28	47	29	2	1	2
	Sb_MNN	1022	0.000	0.883	1040	1010	1039	1011	2	1	2
	Sb_MNN1	1032	0.000	0.866	1040	1010	1039	1011	0	1	2
Argon Ar 18	Ar2p	241	1.231	0.962	255	235	254	236	3	1	2
	Ar2s	319	0.494	0.321	332	312	331	313	0	1	2
	Ar_LMM	1272	0.000	0.266	1285	1260	1284	1261	0	1	2
Arsenic As 33	As2p1	1362	1.232	0.069	1372	1352	1371	1353	2	1	2
	As2p3	1326	2.464	0.525	1340	1320	1339	1321	2	1	2
	As3d	44	0.741	0.713	56	36	55	37	3	1	2
	As3p	142	1.341	0.577	162	137	161	138	0	1	2
	As3s	205	0.350	0.577	215	195	214	196	0	1	2
	As_LMM	266	0.000	0.340	284	259	283	260	2	1	2
	As_LMM1	230	0.000	0.628	250	220	249	221	0	1	2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

## B: XPS Sensitivity Factors

Element			Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡
					Area	Height	High	Low	High	Low			
Barium	Ba	56	Ba3d3	795	5.001	4.835	805	785	804	786	2	1	2
			Ba3d5	780	7.343	6.971	794	774	793	775	3	1	2
			Ba4d	90	3.224	1.852	105	85	104	86	2	1	2
			Ba4p3	177	0.620	0.554	187	167	186	168	0	1	2
			Ba_MNN	886	0.000	0.682	930	860	929	861	2	1	2
			Ba_MNN1	900	0.000	0.962	930	860	929	861	0	1	2
Beryllium	Be	4	Be1s	113	0.080	0.080	127	107	126	108	3	1	2
Bismuth	Bi	83	Bi4d3	467	1.952	0.792	477	457	476	458	2	1	2
			Bi4d5	443	2.907	1.163	462	437	461	438	2	1	2
			Bi4f	159	9.848	5.656	172	152	171	153	3	1	2
			Bi4f5	164	4.515	4.515	174	154	173	155	2	1	2
			Bi4f7	159	5.656	5.656	178	153	177	154	2	1	2
			Bi4p3	681	1.606	0.412	691	671	690	672	2	1	2
			Bi5d	26	1.551	0.916	40	20	39	21	0	1	2
Boron	B	5	B1s	191	0.171	0.171	202	182	201	183	3	1	2
			B_KLL	1310	0.000	0.006	1325	1290	1324	1291	0	1	2
Bromine	Br	35	Br3d	69	1.149	1.066	83	63	82	64	3	1	2
			Br3p	182	1.502	0.711	198	178	197	179	2	1	2
			Br3p1	189	0.512	0.289	199	179	198	180	0	1	2
			Br3p3	182	0.988	0.711	192	172	191	173	0	1	2
			Br3s	256	0.410	0.178	266	246	265	247	0	1	2
Cadmium	Cd	48	Cd3d3	412	2.858	2.858	422	402	421	403	2	1	2
			Cd3d5	405	4.148	4.148	419	399	418	400	3	1	2
			Cd3p1	652	0.820	0.338	662	642	661	643	2	1	2
			Cd3p3	618	1.682	0.788	633	613	632	614	2	1	2
			Cd3s	772	0.800	0.788	782	762	781	763	0	1	2
			Cd4d	11	0.752	0.582	21	1	20	2	2	1	2
			Cd_MNN	1103	0.000	0.673	1120	1090	1119	1091	2	1	2
			Cd_MNN1	1110	0.000	0.938	1120	1090	1119	1091	0	1	2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

## B: XPS Sensitivity Factors

Element			Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡
					Area	Height	High	Low	High	Low			
Calcium	Ca	20	Ca2p	347	1.927	1.281	361	341	360	342	3	1	2
			Ca2p1	350	0.658	0.585	360	340	359	341	2	1	2
			Ca2p3	347	1.281	1.281	362	342	361	343	2	1	2
			Ca2s	439	0.548	0.303	454	434	453	435	2	1	2
			Ca_LMM	1197	0.000	0.212	1207	1175	1206	1176	0	1	2
Carbon	C	6	C1s	284.8	0.314	0.314	298	278	297	279	3	1	2
			C_KLL	1223	0.000	0.020	1240	1200	1239	1201	2	1	2
Cerium	Ce	58	Ce3d	882	12.000	1.560	916	876	915	877	2	1	2
			Ce3d3	900	5.001	1.052	910	890	909	891	2	1	2
			Ce3d5	882	7.343	1.560	902	872	901	873	3	1	2
			Ce4d	108	2.720	0.817	125	105	124	106	2	1	2
			Ce_MNN	833	0.000	0.838	860	820	859	821	2	1	2
Cesium	Cs	55	Cs3d	724	11.800	6.801	759	719	758	720	3	1	2
			Cs3d3	738	4.805	4.709	748	728	747	729	2	1	2
			Cs3d5	724	6.995	6.801	738	718	737	719	2	1	2
			Cs3p3	997	1.658	0.460	1007	987	1006	988	2	1	2
			Cs4d	75	2.761	1.726	90	70	89	71	2	1	2
			Cs4p3	158	0.620	0.533	168	148	167	149	0	1	2
			Cs_MNN	918	0.000	1.092	950	890	949	891	2	1	2
			Cs_MNN1	931	0.000	0.976	950	890	949	891	0	1	2
Chlorine	Cl	17	Cl2p	199	0.954	0.797	213	193	212	194	3	1	2
			Cl2s	270	0.468	0.316	285	265	284	266	2	1	2
			Cl_LMM	1304	0.000	0.181	1315	1290	1314	1291	0	1	2
Chromium	Cr	24	Cr2p	577	2.488	1.623	607	567	606	568	0	1	2
			Cr2p1	586	0.860	0.860	596	576	595	576	0	1	2
			Cr2p3	577	1.623	1.623	589	569	588	570	3	1	2
			Cr2s	698	0.892	0.109	708	688	707	689	0	1	2
			Cr3p	45	0.200	0.238	58	38	57	39	2	1	2
			Cr3s	77	0.080	0.069	87	67	86	68	0	1	2
			Cr_LMM	959	0.000	0.118	975	945	974	946	0	1	2
			Cr_LMM1	997	0.000	0.361	1015	980	1014	981	0	1	2
			Cr_LMM2	917	0.000	0.366	925	905	924	906	0	1	2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

## B: XPS Sensitivity Factors

Element	Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡	
			Area	Height	High	Low	High	Low				
Cobalt	Co 27	Co2p	781	3.529	2.322	815	765	814	766	0	1	2
		Co2p1	796	1.056	1.008	806	786	805	787	0	1	2
		Co2p3	781	2.113	2.322	795	770	794	771	3	1	2
		Co3p	61	0.486	0.347	75	55	74	56	0	1	2
		Co3s	103	0.170	0.117	113	93	112	94	0	1	2
		Co_LMM	713	0.000	0.000	735	685	734	686	2	1	2
		Co_LMM1	777	0.000	0.438	795	765	794	766	0	1	2
		Co_LMM2	838	0.000	0.302	865	820	864	821	0	1	2
Copper	Cu 29	Cu2p	934	4.395	2.930	974	924	973	925	0	1	2
		Cu2p1	954	1.313	1.152	964	944	963	945	0	1	2
		Cu2p3	934	2.626	2.930	952	927	951	928	3	1	2
		Cu3p	77	0.897	0.552	109	59	109	60	2	1	2
		Cu_LMM	568	0.000	0.129	620	540	619	541	2	1	2
		Cu_LMM1	548	0.000	1.087	560	530	559	531	0	1	2
		Cu_LMM2	640	0.000	0.134	660	620	659	621	0	1	2
		Cu_LMM3	648	0.000	0.189	660	620	659	621	0	1	2
Dysprosium	Dy 66	Dy3d5	1295	7.343	0.000	1305	1285	1304	1286	2	1	2
		Dy4d	154	2.668	2.668	175	145	174	146	3	1	2
		Dy4p3	293	0.750	0.751	306	286	305	287	2	1	2
Erbium	Er 68	Er4d	169	2.650	2.650	180	160	179	161	3	1	2
		Er4p	320	0.741	0.741	335	315	334	316	2	1	2
Europium	Eu 63	Eu3d	1126	12.000	1.890	1185	1110	1184	1111	2	1	2
		Eu3d5	1126	7.343	1.890	1150	1115	1149	1116	3	1	2
		Eu4d	128	2.689	2.689	180	120	179	121	2	1	2
Fluorine	F 9	F1s	686	1.000	1.000	699	679	698	680	3	1	2
		F2s	30	0.056	0.056	42	22	41	23	2	1	2
		F_KLL	832	0.000	0.430	845	820	844	821	2	1	2
		F_KLL1	858	0.000	0.029	870	845	869	846	0	1	2
		F_KLL2	877	0.000	0.028	890	870	889	871	0	1	2
Gadolinium	Gd 64	Gd3d	1186	12.000	0.896	1215	1175	1214	1176	2	1	2
		Gd4d	141	2.683	2.683	167	132	166	133	3	1	2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

## B: XPS Sensitivity Factors

Element	Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡
			Area	Height	High	Low	High	Low			
Gallium Ga 31	Ga2p1	1144	1.376	1.023	1154	1134	1153	1135	2	1	2
	Ga2p3	1117	2.751	2.203	1140	1110	1139	1111	3	1	2
	Ga3d	20	0.438	0.438	34	14	33	15	2	1	2
	Ga3p	105	1.145	0.545	121	101	120	102	0	1	2
	Ga3s	160	0.290	0.438	170	150	169	151	0	1	2
	Ga_LMM	419	0.000	1.008	430	410	429	411	0	1	2
	Ga_LMM1	392	0.000	1.991	405	380	404	381	0	1	2
	Ga_LMM2	487	0.000	0.241	500	460	499	461	0	1	2
	Ga_LMM3	504	0.000	0.239	515	490	514	491	0	1	2
	Ga_LMM4	514	0.000	0.356	520	505	519	506	0	1	2
Germanium Ge 32	Ge2p1	1250	1.368	0.711	1260	1240	1259	1241	2	1	2
	Ge2p3	1219	2.735	1.479	1245	1210	1244	1211	3	1	2
	Ge3d	31	0.535	0.520	45	25	44	26	2	1	2
	Ge3p	124	1.243	0.541	140	120	139	121	0	1	2
	Ge3s	181	0.310	0.541	191	171	190	172	0	1	2
	Ge_LMM	342	0.000	0.915	350	330	349	331	2	1	2
	Ge_LMM1	310	0.000	1.934	320	300	319	301	0	1	2
	Ge_LMM2	412	0.000	0.249	422	402	421	403	0	1	2
	Ge_LMM3	433	0.000	0.247	443	413	442	414	0	1	2
	Ge_LMM4	444	0.000	0.369	464	424	463	425	0	1	2
Gold Au 79	Au4d3	354	1.702	0.790	364	344	363	345	2	1	2
	Au4d5	336	2.513	1.103	355	335	354	336	2	1	2
	Au4f	85	6.805	3.849	99	79	98	80	3	1	2
	Au4f5	89	3.019	3.019	99	79	98	80	2	1	2
	Au4f7	85	3.849	3.849	100	80	99	81	2	1	2
	Au4p1	643	0.382	0.072	653	633	652	634	2	1	2
	Au4p3	547	1.134	0.363	557	537	556	538	2	1	2
Hafnium Hf 72	Hf4d	213	3.052	1.169	243	203	242	204	0	1	2
	Hf4d3	224	1.292	0.853	234	214	233	215	2	1	2
	Hf4d5	213	1.844	1.169	243	203	242	204	2	1	2
	Hf4f	17	2.901	2.405	29	9	28	10	3	1	2
	Hf4p1	437	0.385	0.187	447	427	446	428	0	1	2
	Hf4p3	382	0.810	0.456	392	372	391	373	2	1	2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

## B: XPS Sensitivity Factors

Element	Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡
			Area	Height	High	Low	High	Low			
Holmium	Ho	67	Ho4d	161	2.659	2.659	185	155	184	156	3 1 2
			Ho4p	306	0.746	0.746	320	300	319	301	2 1 2
Indium	In	49	In3d3	453	3.239	3.239	463	443	462	444	2 1 2
			In3d5	445	4.530	4.530	459	439	458	440	3 1 2
			In3p1	704	0.829	0.365	714	694	713	695	2 1 2
			In3p3	666	1.705	0.761	680	660	679	661	2 1 2
			In3s	828	0.830	0.761	838	818	837	819	0 1 2
			In4d	17	0.840	0.761	27	7	26	8	2 1 2
			In_MNN	1076	0.000	0.784	1090	1060	1089	1061	2 1 2
			In_MNN1	1084	0.000	0.769	1090	1060	1089	1061	0 1 2
Iodine	I	53	I3d3	630	4.168	4.168	640	620	639	621	2 1 2
			I3d5	619	6.302	6.302	633	613	632	614	3 1 2
			I3p1	930	0.779	0.211	940	920	939	921	2 1 2
			I3p3	874	1.700	0.476	884	864	883	865	2 1 2
			I4d	50	2.009	1.507	64	44	63	45	2 1 2
			I_MNN	982	0.000	0.784	1000	950	999	951	2 1 2
			I_MNN1	971	0.000	0.808	1000	950	999	951	0 1 2
Iridium	Ir	77	Ir4d3	313	1.518	0.744	323	303	322	304	2 1 2
			Ir4d5	297	2.298	1.124	313	288	312	289	2 1 2
			Ir4f	62	5.484	3.332	75	55	74	56	3 1 2
			Ir4f5	65	2.286	2.496	75	55	74	56	2 1 2
			Ir4f7	62	3.124	3.332	74	54	73	55	2 1 2
			Ir4p1	579	0.389	0.151	589	569	588	570	2 1 2
			Ir4p3	497	1.063	0.577	507	487	506	488	2 1 2
Iron	Fe	26	Fe2p	710	2.946	1.964	740	700	739	701	0 1 2
			Fe2p1	723	0.972	0.972	733	713	732	714	0 1 2
			Fe2p3	710	1.964	1.964	727	702	726	703	3 1 2
			Fe3p	55	0.362	0.292	68	48	67	49	2 1 2
			Fe3s	92	0.140	0.243	102	82	101	83	0 1 2
			Fe_LMM	784	0.000	0.506	795	770	794	771	2 1 2
			Fe_LMM1	839	0.000	0.486	850	820	849	821	0 1 2
			Fe_LMM2	888	0.000	0.401	900	850	899	851	0 1 2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

## B: XPS Sensitivity Factors

Element			Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡
					Area	Height	High	Low	High	Low			
Krypton Kr 36	Kr	36	Kr3d	88	1.400	1.249	102	82	101	83	3	1	2
			Kr3p	208	1.601	0.781	230	205	229	206	0	1	2
			Kr3p1	216	0.533	0.781	230	205	229	206	0	1	2
			Kr3p3	208	1.068	0.781	230	205	229	206	0	1	2
Lanthanum La 57	La	57	La3d	834	12.000	5.135	867	827	866	828	2	1	2
			La3d3	851	5.001	3.316	861	841	860	842	2	1	2
			La3d5	834	7.343	5.135	850	825	849	826	3	1	2
			La4d	101	2.730	2.730	115	95	114	96	2	1	2
			La4p3	195	0.650	0.890	205	185	204	186	0	1	2
			La_MNN	867	0.000	1.907	880	840	879	841	2	1	2
Lead Pb 82	Pb	82	Pb4d3	435	1.868	0.957	445	425	444	426	2	1	2
			Pb4d5	413	2.774	1.180	432	407	431	408	2	1	2
			Pb4f	138	9.000	5.131	152	132	151	133	3	1	2
			Pb4f5	143	3.820	4.289	153	133	152	134	2	1	2
			Pb4f7	138	5.172	5.131	150	125	149	126	2	1	2
			Pb4p3	645	1.175	0.392	655	635	654	636	2	1	2
			Pb5d	19	1.414	0.848	34	14	33	15	0	1	2
Lithium Li 3	Li	3	Li1s	56	0.028	0.028	71	51	70	52	3	1	2
Lutetium Lu 71	Lu	71	Lu4d	197	2.617	2.617	218	193	217	194	2	1	2
			Lu4f	7	0.000	0.000	20	0	19	1	3	1	2
			Lu4p1	413	0.385	0.727	423	403	422	404	2	1	2
			Lu4p3	359	0.800	0.727	374	354	373	355	2	1	2
			Lu4s	509	0.420	0.727	519	499	518	500	0	1	2
Magnesium Mg 12	Mg	12	Mg1s	1305	1.035	0.976	1317	1297	1316	1298	3	1	2
			Mg2p	51	0.167	0.167	64	44	63	45	2	1	2
			Mg2s	90	0.274	0.206	104	84	103	85	2	1	2
			Mg_KLL	305	0.000	2.627	318	298	317	299	2	1	2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

## B: XPS Sensitivity Factors

Element	Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡
			Area	Height	High	Low	High	Low			
Manganese Mn 25	Mn2p	641	2.688	1.757	672	632	671	633	0	1	2
	Mn2p1	652	0.923	0.923	662	642	661	643	0	1	2
	Mn2p3	641	1.757	1.757	654	634	653	635	3	1	2
	Mn3p	48	0.260	0.265	63	43	62	44	2	1	2
	Mn3s	83	0.110	0.219	93	53	92	54	0	1	2
	Mn_LMM	900	0.000	0.347	920	890	919	891	2	1	2
	Mn_LMM1	852	0.000	0.648	870	840	869	841	0	1	2
	Mn_LMM2	944	0.000	0.232	960	920	959	921	0	1	2
Mercury Hg 80	Hg4d3	379	1.801	0.840	389	369	388	370	2	1	2
	Hg4d5	359	2.607	1.152	377	352	376	353	2	1	2
	Hg4f	100	7.512	4.302	115	95	114	96	3	1	2
	Hg4f5	104	3.204	3.204	114	94	113	95	2	1	2
	Hg4f7	100	4.302	4.302	115	90	114	91	2	1	2
	Hg4p3	577	1.406	0.476	587	567	586	568	2	1	2
Molybdenum Mo 42	Mo3d	230	3.544	2.243	242	222	241	223	3	1	2
	Mo3d3	233	1.403	1.467	243	223	242	224	2	1	2
	Mo3d5	230	2.139	2.243	243	223	242	224	2	1	2
	Mo3p1	413	0.708	0.413	423	403	422	404	2	1	2
	Mo3p3	396	1.393	0.869	410	390	409	391	2	1	2
	Mo3s	508	0.620	0.135	518	498	517	499	0	1	2
	Mo4p	36	0.517	0.135	46	26	45	27	0	1	2
Neodymium Nd 60	Nd3d	980	12.000	4.373	1025	970	1024	971	2	1	2
	Nd3d5	981	7.343	4.373	1000	970	999	971	3	1	2
	Nd4d	120	2.708	2.708	133	113	132	114	2	1	2
Neon Ne 10	Ne1s	863	1.215	1.215	876	856	875	857	3	1	2
	Ne2s	41	0.098	0.098	55	35	54	36	0	1	2
	Ne_KLL	669	0.000	0.461	675	655	674	656	0	1	2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

## B: XPS Sensitivity Factors

Element	Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡	
			Area	Height	High	Low	High	Low				
Nickel	Ni 28	Ni2p	855	3.702	2.468	894	844	893	845	0	1	2
		Ni2p1	873	1.154	1.191	883	863	882	864	0	1	2
		Ni2p3	855	2.309	2.468	873	848	872	849	3	1	2
		Ni3p	67	0.693	0.416	80	60	79	61	2	1	2
		Ni3s	112	0.200	0.136	122	102	121	103	0	1	2
		Ni_LMM	641	0.000	1.047	660	610	659	611	2	1	2
		Ni_LMM1	712	0.000	0.586	725	690	724	691	0	1	2
		Ni_LMM2	778	0.000	0.305	785	750	784	751	0	1	2
Niobium	Nb 41	Nb3d	206	3.127	2.046	217	197	216	198	3	1	2
		Nb3d3	209	1.249	1.314	219	199	218	200	2	1	2
		Nb3d5	206	1.876	2.046	217	197	216	198	2	1	2
		Nb3p1	379	0.660	0.432	389	369	388	370	2	1	2
		Nb3p3	364	1.330	0.871	377	357	376	356	2	1	2
		Nb3s	470	0.590	0.149	480	460	479	461	0	1	2
		Nb4p	31	0.505	0.149	41	21	40	22	0	1	2
Nitrogen	N 7	N1s	402	0.499	0.499	411	391	410	392	3	1	2
		N_KLL	1107	0.000	0.036	1090	1120	1089	1121	0	1	2
Osmium	Os 76	Os4d	279	3.653	1.134	312	272	311	273	0	1	2
		Os4d3	294	1.439	0.801	304	284	303	285	2	1	2
		Os4d5	279	2.205	1.134	312	272	311	273	2	1	2
		Os4f	52	4.880	3.067	66	46	65	47	3	1	2
		Os4p1	549	0.374	0.110	559	539	558	540	2	1	2
		Os4p3	475	0.995	0.412	485	465	484	466	2	1	2
Oxygen	O 8	O1s	531	0.733	0.733	543	523	542	524	3	1	2
		O2s	23	0.035	0.035	35	15	34	16	0	1	2
		O_KLL	978	0.000	0.171	990	960	989	961	2	1	2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

## B: XPS Sensitivity Factors

Element	Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡
			Area	Height	High	Low	High	Low			
Palladium Pd 46	Pd3d	337	5.637	3.309	350	330	349	331	3	1	2
	Pd3d3	342	2.323	2.323	352	332	351	333	2	1	2
	Pd3d5	337	3.309	3.309	352	332	351	333	2	1	2
	Pd3p1	561	0.787	0.404	571	551	570	552	2	1	2
	Pd3p3	534	1.586	0.821	548	528	547	529	2	1	2
	Pd3s	671	0.740	0.821	681	661	680	662	0	1	2
	Pd4p	52	0.570	0.821	62	42	61	43	0	1	2
	Pd_MNN	1159	0.000	0.942	1170	1140	1169	1141	0	1	2
Phosphorus P 15	P2p	133	0.525	0.485	143	123	142	124	3	1	2
	P2s	191	0.380	0.276	205	185	204	186	2	1	2
Platinum Pt 78	Pt4d3	333	1.596	0.614	343	323	342	324	2	1	2
	Pt4d5	316	2.377	1.114	333	308	332	309	2	1	2
	Pt4f	73	6.080	3.524	86	66	85	67	3	1	2
	Pt4f5	76	2.553	2.553	86	66	85	67	2	1	2
	Pt4f7	73	3.524	3.524	88	68	87	69	2	1	2
	Pt4p3	521	1.083	0.413	531	511	530	512	2	1	2
	Pt_NNN	1317	0.000	0.000	1350	1300	1349	1301	0	1	2
Potassium K 19	K2p	293	1.552	1.039	307	287	306	288	3	1	2
	K2p1	296	0.512	0.512	306	286	305	287	2	1	2
	K2p3	293	1.039	1.039	307	287	306	288	2	1	2
	K2s	378	0.517	0.312	392	372	391	373	0	1	2
	K_LMM	1239	0.000	0.304	1250	1230	1249	1231	0	1	2
Praseodymium Pr 59	Pr3d	930	12.000	6.335	970	920	969	921	2	1	2
	Pr3d5	932	7.343	6.335	957	927	956	928	3	1	2
	Pr4d	114	2.715	2.715	127	107	126	108	2	1	2
Rhenium Re 75	Re4d	263	3.491	1.142	295	255	294	256	0	1	2
	Re4d3	277	1.374	0.794	287	267	286	268	2	1	2
	Re4d5	263	2.107	1.142	295	255	294	256	2	1	2
	Re4f	43	4.339	2.939	55	35	54	36	3	1	2
	Re4p1	521	0.368	0.123	531	511	530	512	2	1	2
	Re4p3	449	0.962	0.429	459	439	458	440	2	1	2
	Re4s	628	0.470	0.094	638	618	637	619	0	1	2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

## B: XPS Sensitivity Factors

Element	Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡
			Area	Height	High	Low	High	Low			
Rhodium Rh 45	Rh3d	309	5.092	2.981	322	302	321	303	3	1	2
	Rh3d3	314	2.106	2.106	324	304	323	305	2	1	2
	Rh3d5	309	2.816	2.816	324	304	323	305	2	1	2
	Rh3p1	522	0.770	0.413	532	512	531	513	2	1	2
	Rh3p3	498	1.560	0.836	513	493	512	494	2	1	2
	Rh3s	629	0.710	0.836	639	619	638	620	0	1	2
	Rh4p	48	0.570	0.836	58	38	57	39	0	1	2
	Rh_MNN	1185	0.000	0.724	1205	1170	1204	1171	0	1	2
Rubidium Rb 37	Rb3d	110	1.673	1.455	125	105	124	106	3	1	2
	Rb3p	238	1.669	0.860	260	235	259	236	0	1	2
	Rb3p1	247	0.550	0.422	257	237	256	238	2	1	2
	Rb3p3	238	1.117	0.860	260	235	259	236	2	1	2
	Rb3s	322	0.470	0.222	332	312	331	313	0	1	2
Ruthenium Ru 44	Ru3d	282	4.529	2.705	295	275	294	276	3	1	2
	Ru3d3	286	1.821	1.821	296	276	295	277	2	1	2
	Ru3d5	282	2.705	2.705	297	277	296	278	2	1	2
	Ru3p1	485	0.740	0.410	495	475	494	476	2	1	2
	Ru3p3	463	1.496	0.840	478	458	477	459	2	1	2
	Ru3s	586	0.680	0.840	596	576	595	577	0	1	2
	Ru4p	43	0.550	0.840	53	33	52	34	0	1	2
	Ru_MNN	1212	0.000	0.510	1230	1200	1229	1201	0	1	2
Samarium Sm 62	Sm3d3	1108	5.001	2.694	1130	1091	1129	1092	2	1	2
	Sm3d5	1083	7.343	2.309	1100	1065	1099	1066	3	1	2
	Sm4d	132	2.694	2.694	147	127	146	128	2	1	2
Scandium Sc 21	Sc2p	402	1.959	1.306	414	394	413	395	3	1	2
	Sc2p1	407	0.651	0.497	417	397	416	398	2	1	2
	Sc2p3	402	1.306	1.306	417	397	416	398	2	1	2
	Sc2s	501	0.564	0.293	516	496	515	497	0	1	2
	Sc_LMM	1149	0.000	0.175	1160	1135	1159	1136	0	1	2
	Sc_LMM1	1118	0.000	0.375	1128	1100	1127	1101	0	1	2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

## B: XPS Sensitivity Factors

Element			Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡
					Area	Height	High	Low	High	Low			
Selenium	Se	34	Se3d	56	0.821	0.640	69	49	68	50	3	1	2
			Se3p1	169	0.498	0.064	179	159	178	160	0	1	2
			Se3p3	163	0.996	0.296	173	153	172	154	0	1	2
			Se3s	232	0.380	0.000	242	222	241	223	0	1	2
			Se_LMM	300	0.000	1.128	182	157	181	158	2	1	2
			Se_LMM1	184	0.000	0.500	202	177	201	178	0	1	2
			Se_LMM2	143	0.000	2.355	163	133	162	134	0	1	2
			Se_LMM3	259	0.000	0.322	279	249	278	250	0	1	2
			Se_LMM4	288	0.000	0.397	308	278	307	279	0	1	2
Silicon	Si	14	Si2p	102	0.368	0.341	114	94	113	95	3	1	2
			Si2s	153	0.347	0.254	165	145	164	146	2	1	2
Silver	Ag	47	Ag3d	368	6.277	3.742	382	362	381	363	3	1	2
			Ag3d3	374	2.527	2.527	374	354	373	355	2	1	2
			Ag3d5	368	3.742	3.742	384	364	383	365	2	1	2
			Ag3p1	604	0.796	0.435	614	594	613	595	2	1	2
			Ag3p3	573	1.649	0.814	585	565	584	566	2	1	2
			Ag3s	719	0.770	0.814	729	709	728	710	2	1	2
			Ag4d	5	0.664	2.422	15	-5	14	-4	2	1	2
			Ag4p	60	0.580	0.814	70	50	69	51	2	1	2
			Ag4s	98	0.178	0.814	108	88	107	89	2	1	2
			Ag_MNN	1129	0.000	0.750	1145	1120	1144	1121	2	1	2
			Ag_MNN1	1135	0.000	0.946	1145	1120	1144	1121	0	1	2
Sodium	Na	11	Na1s	1072	1.102	1.102	1086	1066	1085	1067	3	1	2
			Na2p	31	0.084	0.070	41	21	40	22	0	1	2
			Na2s	64	0.180	0.166	78	58	77	59	0	1	2
			Na_KLL	493	0.000	1.440	520	488	519	489	2	1	2
			Na_KLL1	532	0.000	0.330	545	528	544	529	0	1	2
Strontium	Sr	38	Sr3d	133	1.992	1.669	153	128	152	129	3	1	2
			Sr3p	269	1.747	0.873	291	266	290	267	0	1	2
			Sr3p1	280	0.579	0.416	290	270	289	271	2	1	2
			Sr3p3	269	1.164	0.873	291	266	290	267	2	1	2
			Sr3s	358	0.500	0.146	368	348	367	349	0	1	2
			Sr4p	21	0.461	0.146	31	11	30	12	0	1	2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

## B: XPS Sensitivity Factors

Element	Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡
			Area	Height	High	Low	High	Low			
Sulfur      S    16	S2p	165	0.717	0.650	175	155	174	156	3	1	2
	S2s	229	0.426	0.309	242	222	241	223	2	1	2
	S_LMM	1336	0.000	0.000	1350	1320	1349	1321	0	1	2
Tantalum    Ta   73	Ta4d	229	3.224	1.160	260	220	259	221	0	1	2
	Ta4d3	241	1.282	0.769	251	231	250	232	2	1	2
	Ta4d5	229	1.934	1.160	260	220	259	221	2	1	2
	Ta4f	25	3.384	2.665	37	17	36	16	3	1	2
	Ta4p1	464	0.391	0.161	474	454	473	455	2	1	2
	Ta4p3	403	0.820	0.475	413	393	412	394	2	1	2
	Ta4s	566	0.440	0.131	576	556	575	557	0	1	2
Tellurium   Te   52	Te3d3	585	4.088	4.088	595	575	594	576	2	1	2
	Te3d5	575	5.850	5.850	587	567	586	568	3	1	2
	Te3p1	873	0.794	0.397	883	863	882	864	2	1	2
	Te3p3	822	1.750	0.875	832	812	831	813	2	1	2
	Te4d	43	1.721	1.358	57	37	56	38	2	1	2
	Te_MNN	995	0.000	0.883	1015	985	1014	986	2	1	2
	Te_MNN1	1005	0.000	1.011	1015	985	1014	986	0	1	2
Terbium   Tb   65	Tb3d	1244	12.000	0.621	1275	1235	1274	1236	2	1	2
	Tb4d	150	2.672	2.672	170	140	169	141	3	1	2
Thallium   Tl   81	Tl4d3	406	1.765	0.782	416	396	415	395	2	1	2
	Tl4d5	385	2.693	1.137	403	378	402	379	2	1	2
	Tl4f	118	8.334	4.743	132	112	131	113	3	1	2
	Tl4f5	122	3.585	3.585	132	112	131	113	2	1	2
	Tl4f7	118	4.743	4.743	133	113	132	114	2	1	2
	Tl4p3	608	1.164	0.434	618	598	617	599	2	1	2
	Tl5d	13	1.276	0.780	28	8	27	9	0	1	2
Thorium   Th   90	Th4d3	714	2.252	0.783	724	704	723	705	2	1	2
	Th4d5	677	3.524	1.208	695	670	694	671	2	1	2
	Th4f5	344	7.450	7.450	354	334	353	335	2	1	2
	Th4f7	335	9.568	9.568	347	327	346	328	3	1	2
	Th5d	87	2.060	1.236	102	82	101	83	0	1	2
	Th5d3	94	0.822	0.822	104	84	103	85	0	1	2
	Th5d5	87	1.236	1.236	102	82	101	83	0	1	2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

## B: XPS Sensitivity Factors

Element		Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡
				Area	Height	High	Low	High	Low			
Thulium	Tm 69	Tm4d	180	2.637	2.637	185	165	184	166	3	1	2
Tin	Sn 50	Sn3d	488.5	8.288	4.890	500	480	499	481	2	1	2
		Sn3d3	494	3.398	3.398	504	484	503	485	2	1	2
		Sn3d5	486	4.890	4.890	500	480	499	481	3	1	2
		Sn3p1	757	0.824	0.350	767	747	766	748	2	1	2
		Sn3p3	715	1.732	0.734	730	710	729	711	2	1	2
		Sn3s	885	0.870	0.804	895	875	894	876	0	1	2
		Sn4d	25	1.100	0.804	35	15	34	16	2	1	2
		Sn_MNN	1049	0.000	0.814	1070	1040	1069	1041	2	1	2
		Sn_MNN1	1058	0.000	0.902	1070	1040	1069	1041	0	1	2
Titanium	Ti 22	Ti2p	458	2.077	1.385	469	449	468	450	3	1	2
		Ti2p1	464	0.690	0.690	474	454	473	455	2	1	2
		Ti2p3	458	1.385	1.385	476	451	475	452	2	1	2
		Ti2s	565	0.589	0.284	578	558	577	559	2	1	2
		Ti3p	37	0.090	0.210	52	32	51	33	2	1	2
		Ti3s	59	0.030	0.171	70	50	69	51	0	1	2
		Ti_LMM	1068	0.000	0.332	1080	1055	1079	1056	0	1	2
		Ti_LMM1	1098	0.000	0.182	1110	1080	1109	1081	0	1	2
Tungsten	W 74	W4d	245	3.328	1.152	276	236	275	237	0	1	2
		W4d3	257	1.387	0.827	267	247	266	248	2	1	2
		W4d5	245	2.010	1.152	276	236	275	237	2	1	2
		W4f	34	3.863	2.810	46	26	45	27	3	1	2
		W4p1	491	0.386	0.125	501	481	500	482	2	1	2
		W4p3	425	0.830	0.469	435	415	434	416	2	1	2
		W4s	594	0.460	0.118	604	584	603	585	0	1	2
		U4d3	781	2.359	0.836	791	771	790	772	2	1	2
Uranium	U 92	U4d5	739	3.697	1.248	757	732	756	733	2	1	2
		U4f5	391	8.474	8.474	401	381	400	382	2	1	2
		U4f7	380	10.800	10.800	387	372	386	373	3	1	2
		U5d	96	2.189	1.368	110	90	109	91	0	1	2
		U5d3	104	0.818	0.818	114	94	113	95	0	1	2
		U5d5	96	1.368	1.368	110	90	109	91	0	1	2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

## B: XPS Sensitivity Factors

Element	Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡
			Area	Height	High	Low	High	Low			
Vanadium V 23	V2p	515	2.184	1.456	536	511	535	512	0	1	2
	V2p1	523	0.725	0.725	533	513	532	514	0	1	2
	V2p3	515	1.456	1.456	527	507	526	508	3	1	2
	V2s	630	0.688	0.134	640	620	639	621	0	1	2
	V3p	40	0.140	0.224	53	33	52	34	0	1	2
	V3s	66	0.050	0.183	75	55	74	56	0	1	2
	V_LMM	1014	0.000	0.114	1030	1000	1029	1001	0	1	2
	V_LMM1	1048	0.000	0.413	1060	1040	1059	1041	0	1	2
	V_LMM2	977	0.000	0.307	1000	955	999	956	0	1	2
Xenon Xe 54	Xe3d3	685	4.404	4.404	695	675	694	676	2	1	2
	Xe3d5	672	6.670	6.670	684	664	683	665	3	1	2
	Xe4d	63	2.387	1.610	77	57	76	58	2	1	2
	Xe_MNN	955	0.000	1.127	970	920	969	921	2	1	2
Ytterbium Yb 70	Yb4d	185	2.631	2.631	215	165	214	166	3	1	2
	Yb4p1	389	0.385	0.734	405	379	404	380	2	1	2
	Yb4p3	333	0.760	0.734	348	328	347	329	2	1	2
	Yb4s	482	0.410	0.734	492	472	491	473	0	1	2
Yttrium Y 39	Y3d	158	2.343	1.824	171	151	170	152	3	1	2
	Y3p	301	1.833	0.885	323	298	322	299	0	1	2
	Y3p1	313	0.610	0.434	323	303	322	304	2	1	2
	Y3p3	301	1.222	0.885	323	298	322	299	2	1	2
	Y3s	395	0.530	0.143	405	385	404	386	0	1	2
	Y4p	24	0.460	0.143	34	14	33	15	0	1	2
Zinc Zn 30	Zn2p1	1045	1.384	1.253	1055	1035	1054	1036	2	1	2
	Zn2p3	1022	2.768	2.680	1036	1016	1035	1017	3	1	2
	Zn3d	10	0.371	0.549	20	0	19	1	0	1	2
	Zn3p	89	1.029	0.549	104	84	103	85	2	1	2
	Zn3s	140	0.260	0.549	150	130	149	131	0	1	2
	Zn_LMM	495	2.911	0.546	515	480	514	481	2	1	2
	Zn_LMM1	472	0.000	1.919	492	480	491	481	0	1	2
	Zn_LMM2	582	0.000	0.242	600	570	599	571	0	1	2
	Zn_LMM3	573	0.000	0.379	600	570	599	571	0	1	2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

## B: XPS Sensitivity Factors

Element	Transition	Peak	S <sub>x</sub>		Acquisition		Analysis		*	†	‡
			Area	Height	High	Low	High	Low			
Zirconium Zr 40	Zr3d	181	2.767	1.977	194	174	193	175	3	1	2
	Zr3p	331	1.917	0.885	345	325	344	326	0	1	2
	Zr3p1	345	0.635	0.439	355	335	354	336	2	1	2
	Zr3p3	331	1.278	0.885	352	322	351	323	2	1	2
	Zr3s	431	0.560	0.175	441	421	440	422	0	1	2
	Zr4p	28	0.468	0.175	38	18	37	19	0	1	2

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

‡ Background type.

# Appendix C: AES Sensitivity Factors

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Two types of relative sensitivity factors (RSF) are available in MultiPak. One is elemental relative sensitivity factors (ERSF), which are available for all versions. The other is average matrix relative sensitivity factors (AMRSF), which are available for version 9.2 or later. ERSFs are selected at the original installation for compatibility with prior versions. To switch the RSF from ERSF/AMRSF to AMRSF/ERSF, refer to Section 3 "Periodic Table". The sensitivity factors contained in MultiPak's AES database can be modified by the user, as described in Section 3, "Transition Dialog Box." For more information about AES sensitivity factors, refer to Appendix A, "Sensitivity Factors."

## Elemental relative sensitivity factors

These values are valid only for data that have had a 5-point derivative applied to them.

Element	Region	Peak	Sensitivity Factor ( $S_x$ )			Acquisition		Analysis		*	†
			3 keV	5 keV	10 keV	High	Low	High	Low		
Aluminum Al 13	Al1	70	0.317	0.295	0.176	92	32	84	50	0	10
	Al3	70	0.240	0.190	0.150	92	32	84	50	0	10
	Al2	1396	0.075	0.121	0.105	1416	1356	1408	1374	3	15
	Al4	1396	0.110	0.170	0.200	1416	1356	1408	1374	0	15
Antimony Sb 51	Sb1	458	0.738	0.704	0.525	480	420	472	438	3	5
	Sb2	3035	–	0.003	0.007	3047	2987	3039	3005	0	185
Arsenic As 33	As4	97	0.039	0.028	0.017	117.5	57.5	109.5	75.5	0	80
	As3	1118	0.062	0.067	0.029	1139.5	1079.5	1131.5	1097.5	0	45
	As1	1229	0.111	0.124	0.110	1250	1190	1242	1208	3	10
	As2	1264	0.052	0.059	0.053	1285	1225	1277	1243	0	25

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\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor (S <sub>x</sub> )			Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	High	Low	High	Low			
Barium	Ba 56	Ba1	58	0.128	0.109	0.076	79	19	71	37	0	20
		Ba2	76	0.124	0.097	0.065	97	37	89	55	0	20
		Ba3	603	0.080	0.084	0.071	610.5	550.5	602.5	568.5	3	20
		Ba4	674	0.013	0.014	0.012	694	634	686	652	0	115
Beryllium	Be 4	Be1	108	0.270	0.188	0.108	128	68	120	86	3	10
Bismuth	Bi 83	Bi1	105	0.348	0.303	0.212	127	67	119	85	3	5
		Bi2	253	0.023	0.022	0.017	272	212	264	230	0	80
		Bi5	1960	–	0.006	0.007	1957	1897	1949	1915	0	200
		Bi3	2243	0.004	0.014	0.017	2256	2196	2248	2214	0	80
		Bi4	2350	–	0.011	0.012	2365	2305	2357	2323	0	110
Boron	B 5	B1	185	0.239	0.171	0.105	203	143	195	161	3	15
Bromine	Br 35	Br5	55	0.138	0.097	0.073	78	18	70	36	0	20
		Br4	102	0.070	0.055	0.041	126	66	118	84	0	35
		Br3	1267	0.025	0.030	0.030	1288	1228	1280	1246	0	45
		Br1	1393	0.073	0.095	0.103	1413.5	1353.5	1405.5	1371.5	3	15
		Br2	1439	0.045	0.051	0.057	1459.5	1399.5	1451.5	1417.5	0	25
Cadmium	Cd 48	Cd1	379	1.041	0.934	0.701	402	342	394	360	3	5
		Cd2	2694	–	0.006	0.011	2708	2648	2700	2666	0	125
Calcium	Ca 20	Ca1	297	0.249	0.199	0.132	314	254	306	272	3	10
Carbon	C 6	C1	275	0.165	0.128	0.076	291	231	283	249	3	20
Cerium	Ce 58	Ce1	87	0.441	0.316	0.196	109.5	49.5	101.5	67.5	0	5
		Ce2	671	0.061	0.058	0.043	679	619	671	637	3	30
		Ce3	774	0.028	0.027	0.019	778	718	770	736	0	70
Cesium	Cs 55	Cs1	572	0.084	0.083	0.066	579	519	571	537	3	20
		Cs2	632	0.012	0.012	0.009	653	593	645	611	0	145
Chlorine	Cl 17	Cl1	184	3.199	2.182	1.724	206.5	146.5	198.5	164.5	3	5
Chromium	Cr 24	Cr1	491	0.344	0.308	0.226	514	454	506	472	0	5
		Cr2	531	0.404	0.359	0.265	552	492	544	510	3	5
Cobalt	Co 27	Co4	57	0.459	0.351	0.217	78	18	70	36	0	5
		Co3	658	0.109	0.109	0.084	673	613	665	631	0	15
		Co2	718	0.141	0.142	0.109	735	675	727	693	0	10
		Co1	777	0.300	0.299	0.226	798	738	790	756	3	5

\* Peak labeling (e.g., 0 = “none”).

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor (S <sub>x</sub> )			Acquisition		Analysis		*	†
			3 keV	5 keV	10 keV	High	Low	High	Low		
Copper Cu 29	Cu4	66	0.361	0.297	0.197	87	27	79	45	0	5
		778	0.044	0.051	0.045	793	733	785	751	0	30
		842	0.080	0.093	0.081	864.5	804.5	856.5	822.5	0	15
		922	0.260	0.307	0.269	943.5	883.5	935.5	901.5	3	5
Dysprosium Dy 66	Dy1	154	0.125	0.072	0.043	168.5	108.5	160.5	126.5	0	30
		978	0.019	0.018	0.015	979	919	971	937	0	90
		1127	0.025	0.023	0.020	1138	1078	1130	1096	3	70
		1284	0.012	0.011	0.009	1299	1239	1291	1257	0	150
Erbium Er 68	Er1	168	0.089	0.067	0.043	174	114	166	132	0	30
		1060	0.012	0.014	0.014	1065	1005	1057	1023	0	95
		1228	0.018	0.023	0.021	1236	1176	1228	1194	3	65
		1395	0.017	0.022	0.021	1411	1351	1403	1369	0	65
Europium Eu 63	Eu1	107	0.250	0.169	0.109	130	70	122	88	0	10
		140	0.145	0.098	0.063	162	102	154	120	0	20
		860	0.037	0.036	0.032	869	809	861	827	3	40
		988	0.037	0.036	0.032	999	939	991	957	0	45
Flourine F 9	F1	659	0.499	0.717	0.513	680	620	672	638	3	5
Gadolinium Gd 64	Gd1	112	0.157	0.131	0.077	134	74	126	92	0	15
		143	0.190	0.153	0.088	164.5	104.5	156.5	122.5	0	15
		896	0.023	0.029	0.024	907	847	899	865	0	55
		1030	0.024	0.031	0.026	1044	984	1036	1002	3	50
Gallium Ga 31	Ga4	58	0.171	0.130	0.077	80	20	72	38	0	15
		974	0.063	0.073	0.060	996	936	988	954	0	25
		1069	0.246	0.273	0.225	1091	1031	1083	1049	3	5
		1096	0.130	0.137	0.115	1118	1058	1110	1076	0	10
Germanium Ge 32	Ge4	55	0.077	0.063	0.040	78	18	70	36	0	35
		1047	0.038	0.046	0.040	1068.5	1008.5	1060.5	1026.5	0	35
		1150	0.140	0.172	0.149	1171.5	1111.5	1163.5	1129.5	3	10
		1181	0.063	0.079	0.069	1202	1142	1194	1160	0	20

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor (S <sub>x</sub> )			Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	High	Low	High	Low			
Gold	Au 79	Au1	74	0.629	0.532	0.381	96	36	88	54	0	5
		Au2	243	0.048	0.044	0.033	264.5	204.5	256.5	222.5	0	40
		Au6	1522	0.003	0.007	0.008	1524	1464	1516	1482	0	175
		Au5	1771	0.007	0.013	0.015	1789	1729	1781	1747	0	90
		Au3	2022	0.020	0.041	0.049	2040	1980	2032	1998	3	25
		Au4	2107	0.011	0.030	0.038	2125	2065	2117	2083	0	35
Hafnium	Hf 72	Hf1	184	0.134	0.116	0.072	195	135	187	153	0	20
		Hf4	1231	0.007	0.012	0.012	1241	1181	1233	1199	0	115
		Hf3	1427	0.014	0.024	0.023	1433	1373	1425	1391	0	60
		Hf2	1625	0.047	0.075	0.070	1644	1584	1636	1602	3	20
Holmium	Ho 67	Ho1	162	0.098	0.077	0.045	175	115	167	133	0	30
		Ho3	1016	0.015	0.019	0.016	1020	960	1012	978	0	85
		Ho2	1177	0.025	0.031	0.026	1186	1126	1178	1144	3	50
		Ho4	1339	0.015	0.018	0.015	1354	1294	1346	1312	0	85
Indium	In 49	In1	405	0.715	0.586	0.432	428	368	420	386	3	5
		In2	2806	–	0.004	0.007	2818	2758	2810	2776	0	180
Iodine	I 53	I1	510	0.269	0.256	0.287	531	471	523	489	3	5
			519	0.269	0.242	0.256	541	481	533	499	0	5
			562	0.032	0.037	0.037	584.5	524.5	576.5	542.5	0	35
Iridium	Ir 77	Ir1	175	0.082	0.069	0.045	188	128	180	146	0	30
		Ir4	233	0.051	0.044	0.028	254	194	246	212	0	50
		Ir6	1439	0.004	0.009	0.009	1443	1383	1435	1401	0	145
		Ir5	1672	0.010	0.016	0.016	1690	1630	1682	1648	0	85
		Ir2	1909	0.027	0.053	0.055	1926	1866	1918	1884	3	25
		Ir3	1982	0.018	0.040	0.043	2000	1940	1992	1958	0	30
Iron	Fe 26	Fe4	50	0.670	0.515	0.317	73	13	65	31	0	5
		Fe1	600	0.144	0.139	0.103	616	556	608	574	3	15
		Fe2	654	0.212	0.205	0.150	672.5	612.5	664.5	630.5	0	10
		Fe3	705	0.255	0.246	0.178	727.5	667.5	719.5	685.5	0	10
Lanthanum	La 57	La1	83	0.389	0.271	0.168	105	45	97	63	0	10
		La2	634	0.080	0.075	0.059	644	584	636	602	3	25
		La3	732	0.027	0.025	0.019	736.5	676.5	728.5	694.5	0	70

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor (S <sub>x</sub> )			Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	High	Low	High	Low			
Lead	Pb 82	Pb1	97	0.551	0.473	0.311	119	59	111	77	3	5
		Pb2	251	0.033	0.032	0.022	272	212	264	230	0	60
		Pb6	1641	–	0.003	0.004	1638	1578	1630	1596	0	340
		Pb5	1914	0.003	0.008	0.009	1910	1850	1902	1868	0	145
		Pb3	2188	0.005	0.020	0.023	2201	2141	2193	2159	0	60
		Pb4	2288	–	0.001	0.016	2303.5	2243.5	2295.5	2261.5	0	85
Lithium	Li 3	Li1	57	0.120	0.070	0.024	72	12	64	30	3	55
Lutetium	Lu 71	Lu1	182	0.107	0.086	0.052	194	134	186	152	0	25
		Lu4	1188	0.009	0.012	0.010	1198	1138	1190	1156	0	135
		Lu3	1378	0.014	0.020	0.017	1384	1324	1376	1342	0	75
		Lu2	1568	0.040	0.057	0.050	1586	1526	1578	1544	3	25
Magnesium	Mg 12	Mg1	48	0.381	0.283	0.174	71	11	63	29	0	10
		Mg2	1188	0.098	0.121	0.109	1199	1139	1191	1157	3	10
Manganese	Mn 25	Mn4	45	0.508	0.369	0.226	67	7	59	25	0	5
		Mn1	545	0.189	0.173	0.122	561	501	553	519	3	10
		Mn2	592	0.246	0.222	0.161	611	551	603	569	0	10
		Mn3	638	0.189	0.169	0.123	660	600	652	618	0	10
Mercury	Hg 80	Hg1	81	0.518	0.427	0.287	103	43	95	61	3	5
		Hg2	246	0.037	0.032	0.023	268	208	260	226	0	60
		Hg5	1818	0.006	0.011	0.012	1836	1776	1828	1794	0	110
		Hg3	2078	0.018	0.028	0.032	2093	2033	2085	2051	0	40
		Hg4	2166	0.013	0.019	0.024	2184	2124	2176	2142	0	55
Molybdenum	Mo 42	Mo1	190	0.343	0.271	0.170	212	152	204	170	3	10
		Mo3	225	0.302	0.241	0.149	247	187	239	205	0	10
		Mo5	1881	0.003	0.008	0.009	1899	1839	1891	1857	0	145
		Mo2	2044	0.008	0.028	0.031	2062	2002	2054	2020	0	45
		Mo4	2149	0.003	0.013	0.015	2167	2107	2159	2125	0	90
Neodymium	Nd 60	Nd1	96	0.357	0.257	0.166	118	58	110	76	0	10
		Nd2	734	0.057	0.056	0.047	751	691	743	709	3	30
		Nd3	861	0.022	0.022	0.018	863	803	855	821	0	75
Nickel	Ni 28	Ni4	64	0.410	0.321	0.208	84	24	76	42	0	5
		Ni3	718	0.063	0.066	0.053	733	673	725	691	0	25
		Ni2	785	0.103	0.107	0.086	799	739	791	757	0	15
		Ni1	849	0.269	0.281	0.227	871	811	863	829	3	5

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )			Acquisition		Analysis		*	†
			3 keV	5 keV	10 keV	High	Low	High	Low		
Niobium Nb 41	Nb1	170	0.357	0.289	0.190	192.5	132.5	184.5	150.5	3	5
	Nb3	201	0.191	0.153	0.100	223.5	163.5	215.5	181.5	0	15
	Nb5	1787	0.004	0.010	0.011	1787	1727	1779	1745	0	125
	Nb2	1944	0.011	0.026	0.031	1962	1902	1954	1920	0	45
	Nb4	2039	0.007	0.012	0.015	2056	1996	2048	2014	0	90
Nitrogen N 7	N1	389	0.327	0.246	0.161	407	347	399	365	3	10
Osmium Os 76	Os1	180	0.102	0.071	0.046	191	131	183	149	0	30
	Os4	226	0.045	0.031	0.020	247	187	239	205	0	65
	Os6	1396	0.006	0.008	0.008	1402	1342	1394	1360	0	160
	Os5	1622	0.010	0.014	0.014	1640	1580	1632	1598	0	95
	Os2	1850	0.037	0.054	0.055	1869	1809	1861	1827	3	25
	Os3	1920	0.024	0.037	0.038	1938	1878	1930	1896	0	35
Oxygen O 8	O1	510	0.338	0.296	0.212	532	472	524	490	3	5
	O2	510	0.258	0.247	0.220	532	472	524	490	0	5
Palladium Pd 46	Pd2	283	0.152	0.132	0.094	300	240	292	258	0	15
	Pd1	333	0.882	0.768	0.547	352.5	292.5	344.5	310.5	3	5
	Pd5	2282	–	0.004	0.005	2300	2240	2292	2258	0	270
	Pd3	2476	–	0.012	0.017	2492	2432	2484	2450	0	75
	Pd4	2633	–	0.005	0.008	2650	2590	2642	2608	0	160
Phosphorus P 15	P1	123	0.828	0.613	0.371	145.5	85.5	137.5	103.5	3	5
	P2	1862	0.024	0.046	0.049	1880	1820	1872	1838	0	25
Platinum Pt 78	Pt1	70	0.513	0.393	0.296	89	29	81	47	3	5
	Pt2	173	0.043	0.035	0.028	195	135	187	153	0	50
	Pt3	241	0.042	0.034	0.026	261.5	201.5	253.5	219.5	0	50
	Pt7	1484	0.003	0.007	0.008	1487	1427	1479	1445	0	175
	Pt6	1725	0.008	0.012	0.015	1743	1683	1735	1701	0	90
	Pt4	1969	0.022	0.042	0.051	1987	1927	1979	1945	3	25
	Pt5	2048	0.016	0.035	0.043	2067	2007	2059	2025	0	30
Potassium K 19	K1	252	0.300	0.255	0.192	272	212	264	230	3	5

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )			Acquisition		Analysis		*	†
			3 keV	5 keV	10 keV	High	Low	High	Low		
Praseodymium Pr 59	Pr1	91	0.361	0.266	0.165	113.5	53.5	105.5	71.5	0	10
	Pr2	696	0.049	0.049	0.038	714	654	706	672	3	35
	Pr3	817	0.021	0.020	0.015	820	760	812	778	0	85
Rhenium Re 75	Re1	179	0.155	0.126	0.080	188	128	180	146	0	15
	Re4	218	0.058	0.046	0.029	240	180	232	198	0	45
	Re6	1354	0.007	0.012	0.011	1361	1301	1353	1319	0	120
	Re5	1572	0.012	0.019	0.019	1590	1530	1582	1548	0	70
	Re2	1793	0.041	0.072	0.070	1812	1752	1804	1770	3	20
	Re3	1858	0.025	0.045	0.044	1877	1817	1869	1835	0	30
Rhodium Rh 45	Rh2	259	0.222	0.191	0.140	278	218	270	236	0	10
	Rh1	305	0.848	0.725	0.530	326	266	318	284	3	5
	Rh5	2180	–	0.004	0.006	2197	2137	2189	2155	0	230
	Rh3	2366	–	0.011	0.019	2381	2321	2373	2339	0	70
	Rh4	2507	–	0.005	0.010	2525	2465	2517	2483	0	135
Rubidium Rb 37	Rb5	78	0.053	0.040	0.029	98.5	38.5	90.5	56.5	0	45
	Rb4	107	0.025	0.018	0.013	128.5	68.5	120.5	86.5	0	105
	Rb3	1433	0.003	0.005	0.006	1438	1378	1430	1396	0	210
	Rb1	1561	0.012	0.017	0.022	1579	1519	1571	1537	3	60
	Rb2	1620	0.006	0.008	0.011	1639	1579	1631	1597	0	125
Ruthenium Ru 44	Ru2	235	0.216	0.186	0.114	255	195	247	213	0	10
	Ru1	277	0.574	0.495	0.302	299	239	291	257	3	5
	Ru5	2078	–	0.006	0.006	2063	2003	2055	2021	0	210
	Ru3	2256	–	0.019	0.023	2273	2213	2265	2231	0	60
	Ru4	2385	–	0.009	0.011	2401	2341	2393	2359	0	120
Samarium Sm 62	Sm1	103	0.214	0.160	0.104	125.5	65.5	117.5	83.5	0	15
	Sm3	135	0.109	0.078	0.047	145.5	85.5	137.5	103.5	0	30
	Sm2	814	0.036	0.038	0.031	826	766	818	784	3	45
	Sm4	940	0.026	0.028	0.022	952	892	944	910	0	60
Scandium Sc 21	Sc1	343	0.305	0.250	0.168	362	302	354	320	3	10
	Sc2	370	0.322	0.264	0.176	393	333	385	351	0	10

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )			Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	High	Low	High	Low			
Selenium Se 34	Se5	47	0.027	0.022	0.024	69	9	61	27	2	55	
		Se4	104	0.031	0.024	0.010	122	62	114	80	0	140
		Se3	1192	0.020	0.027	0.008	1213	1153	1205	1171	0	160
		Se1	1311	0.074	0.097	0.032	1331	1271	1323	1289	3	40
		Se2	1352	0.038	0.045	0.016	1372	1312	1364	1330	0	85
Silicon Si 14	Si1	96	0.414	0.403	0.249	118	58	110	76	0	5	
		Si3	96	0.158	0.138	0.115	118	58	110	76	0	5
		Si2	1621	0.034	0.069	0.071	1640	1580	1632	1598	3	20
		Si4	1621	0.063	0.101	0.121	1640	1580	1632	1598	0	20
Silver Ag 47	Ag1	359	1.000	0.878	0.634	376.5	316.5	368.5	334.5	3	5	
		Ag4	2381	–	0.003	0.005	2399	2339	2391	2357	0	285
		Ag2	2583	–	0.008	0.015	2598	2538	2590	2556	0	90
		Ag3	2755	–	0.003	0.007	2771	2711	2763	2729	0	200
Sodium Na 11	Na1	996	0.081	0.087	0.076	1011	951	1003	969	3	20	
Strontium Sr 38	Sr4	114	0.057	0.040	0.029	135	75	127	93	0	45	
		Sr3	1516	0.005	0.006	0.007	1520	1460	1512	1478	0	190
		Sr1	1651	0.016	0.023	0.027	1665	1605	1657	1623	3	50
		Sr2	1718	0.007	0.009	0.011	1731	1671	1723	1689	0	125
Sulfur S 16	S1	153	1.277	1.041	0.652	174.5	114.5	166.5	132.5	3	5	
		S2	2119	0.013	0.023	0.030	2136	2076	2128	2094	0	45
Tantalum Ta 73	Ta1	183	0.175	0.145	0.100	193	133	185	151	0	15	
		Ta4	1271	0.008	0.012	0.013	1280	1220	1272	1238	0	100
		Ta3	1475	0.014	0.024	0.026	1479	1419	1471	1437	0	50
		Ta2	1680	0.046	0.075	0.080	1699	1639	1691	1657	3	15
Tellurium Te 52	Te1	486	0.477	0.437	0.337	507	447	499	465	3	5	
Terbium Tb 65	Tb1	116	0.120	0.067	0.040	139	79	131	97	0	35	
		Tb3	150	0.147	0.079	0.045	167	107	159	125	0	30
		Tb4	937	0.027	0.023	0.018	943	883	935	901	0	75
		Tb2	1078	0.030	0.027	0.021	1091	1031	1083	1049	3	65
		Tb5	1230	0.012	0.009	0.007	1247	1187	1239	1205	0	190

\* Peak labeling (e.g., 0 = "none").

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### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor (S <sub>x</sub> )			Acquisition		Analysis		*	†
			3 keV	5 keV	10 keV	High	Low	High	Low		
Thallium Tl 81	Tl1	90	0.584	0.531	0.332	111.5	51.5	103.5	69.5	3	5
	Tl2	250	0.032	0.031	0.020	270	210	262	228	0	70
	Tl6	1601	–	0.004	0.004	1600	1540	1592	1558	0	330
	Tl5	1865	0.005	0.009	0.009	1863	1803	1855	1821	0	145
	Tl3	2132	0.009	0.024	0.025	2147	2087	2139	2105	0	55
	Tl4	2227	0.006	0.016	0.018	2243	2183	2235	2201	0	75
Thorium Th 90	Th1	69	0.537	0.435	0.286	91.5	31.5	83.5	49.5	3	5
	Th2	249	0.069	0.066	0.049	271.5	211.5	263.5	229.5	0	25
	Th5	2296	–	0.002	0.003	2311	2251	2303	2269	0	420
	Th3	2634	–	0.005	0.007	2645	2585	2637	2603	0	200
	Th4	2789	–	0.003	0.005	2803	2743	2795	2761	0	280
Thulium Tm 69	Tm1	170	0.119	0.085	0.057	179	119	171	137	3	25
	Tm4	1100	0.015	0.017	0.016	1108	1048	1100	1066	0	85
	Tm3	1278	0.022	0.024	0.024	1285	1225	1277	1243	0	55
	Tm2	1452	0.033	0.040	0.038	1469	1409	1461	1427	3	35
Tin Sn 50	Sn1	432	0.688	0.643	0.465	454	394	446	412	3	5
	Sn2	2919	–	0.003	0.006	2933	2873	2925	2891	0	215
Titanium Ti 22	Ti1	390	0.326	0.274	0.188	408	348	400	366	0	5
	Ti2	421	0.518	0.438	0.296	444	384	436	402	3	5
Tungsten W 74	W1	182	0.175	0.141	0.091	193	133	185	151	0	15
	W5	210	0.036	0.028	0.019	232	172	224	190	0	70
	W4	1312	0.010	0.014	0.014	1320	1260	1312	1278	0	100
	W3	1524	0.017	0.024	0.023	1527	1467	1519	1485	0	60
	W2	1737	0.050	0.080	0.080	1755	1695	1747	1713	3	15
Uranium U 92	U1	77	0.888	0.654	0.452	99.5	39.5	91.5	57.5	3	5
	U2	284	0.191	0.166	0.132	307	247	299	265	0	10
	U5	2414	–	0.003	0.004	2429	2369	2421	2387	0	330
	U3	2764	–	0.004	0.008	2780	2720	2772	2738	0	165
	U4	2940	–	0.004	0.007	2955	2895	2947	2913	0	200
Vanadium V 23	V1	440	0.281	0.247	0.176	457	397	449	415	0	10
	V2	475	0.445	0.387	0.272	497	437	489	455	3	5

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor (S <sub>x</sub> )			Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	High	Low	High	Low			
Ytterbium Yb 70	Yb1	174	0.094	0.068	0.052	187	127	179	145	0	25	
		Yb4	1141	0.009	0.011	0.012	1155	1095	1147	1113	0	115
		Yb3	1329	0.013	0.016	0.018	1334	1274	1326	1292	0	75
		Yb2	1511	0.033	0.042	0.046	1526	1466	1518	1484	3	30
Yttrium Y 39	Y1	132	0.157	0.127	0.075	155.5	95.5	147.5	113.5	0	20	
		Y4	1606	0.004	0.008	0.008	1608	1548	1600	1566	0	160
		Y2	1748	0.014	0.029	0.029	1764	1704	1756	1722	3	45
		Y3	1823	0.007	0.013	0.013	1840	1780	1832	1798	0	105
Zinc Zn 30	Zn4	64	0.328	0.261	0.183	86	26	78	44	0	5	
		Zn3	839	0.037	0.041	0.038	853	793	845	811	0	35
		Zn2	908	0.078	0.088	0.083	930.5	870.5	922.5	888.5	0	15
		Zn1	997	0.257	0.296	0.278	1018	958	1010	976	3	5
Zirconium Zr 40	Zr1	151	0.369	0.298	0.204	173.5	113.5	165.5	131.5	3	5	
		Zr4	1695	0.007	0.012	0.015	1697	1637	1689	1655	0	90
		Zr2	1844	0.018	0.036	0.043	1861	1801	1853	1819	0	30
		Zr3	1929	0.006	0.016	0.020	1946	1886	1938	1904	0	65

### relative sensitivity factors for SCA

These values are valid only for data that have had a 5-point derivative applied to them.

Element	Region	Peak	Sensitivity Factor (S <sub>x</sub> )			Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	High	Low	High	Low			
Aluminum Al 13	Al1	70	0.548	0.510	0.304	92	32	84	50	0	10	
		Al3	70	0.415	0.329	0.259	92	32	84	50	0	10
		Al2	1396	0.089	0.144	0.125	1416	1356	1408	1374	3	15
		Al4	1396	0.131	0.202	0.238	1416	1356	1408	1374	0	15
Antimony Sb 51	Sb1	458	0.846	0.807	0.602	480	420	472	438	3	5	
Arsenic As 33	As4	97	0.064	0.046	0.028	117.5	57.5	109.5	75.5	0	80	
		As3	1118	0.070	0.075	0.033	1139.5	1079.5	1131.5	1097.5	0	45

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

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### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )			Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	High	Low	High	Low			
	As1	1229	0.128	0.143	0.126	1250	1190	1242	1208	3	10	
		As2	0.060	0.068	0.061	1285	1225	1277	1243	0	25	
Barium	Ba 56	Ba1	58	0.227	0.193	0.135	79	19	71	37	0	20
		Ba2	76	0.212	0.166	0.111	97	37	89	55	0	20
		Ba3	603	0.087	0.092	0.078	610.5	550.5	602.5	568.5	3	20
		Ba4	674	0.014	0.015	0.013	694	634	686	652	0	115
Beryllium	Be 4	Be1	108	0.435	0.303	0.174	128	68	120	86	3	10
Bismuth	Bi 83	Bi1	105	0.563	0.491	0.343	127	67	119	85	3	5
		Bi2	253	0.030	0.029	0.023	272	212	264	230	0	80
		Bi5	1960	–	0.007	0.008	1957	1897	1949	1915	0	200
		Bi3	2243	0.004	0.013	0.016	2256	2196	2248	2214	0	80
		Bi4	2350	–	0.009	0.010	2365	2305	2357	2323	0	110
Boron	B 5	B1	185	0.343	0.245	0.151	203	143	195	161	3	15
Bromine	Br 35	Br5	55	0.246	0.173	0.130	78	18	70	36	0	20
		Br4	102	0.114	0.090	0.067	126	66	118	84	0	35
		Br3	1267	0.029	0.035	0.035	1288	1228	1280	1246	0	45
		Br1	1393	0.087	0.113	0.122	1413.5	1353.5	1405.5	1371.5	3	15
		Br2	1439	0.054	0.061	0.068	1459.5	1399.5	1451.5	1417.5	0	25
Cadmium	Cd 48	Cd1	379	1.246	1.118	0.839	402	342	394	360	3	5
Calcium	Ca 20	Ca1	297	0.317	0.253	0.168	314	254	306	272	3	10
Carbon	C 6	C1	275	0.214	0.166	0.099	291	231	283	249	3	20

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### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )			Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	High	Low	High	Low			
Cerium	Ce 58	Ce1	87	0.738	0.529	0.328	109.5	49.5	101.5	67.5	0	5
		Ce2	671	0.066	0.063	0.047	679	619	671	637	3	30
		Ce3	774	0.030	0.029	0.020	778	718	770	736	0	70
Cesium	Cs 55	Cs1	572	0.093	0.091	0.073	579	519	571	537	3	20
		Cs2	632	0.013	0.013	0.010	653	593	645	611	0	145
Chlorine	Cl 17	Cl1	184	4.592	3.132	2.475	206.5	146.5	198.5	164.5	3	5
Chromium	Cr 24	Cr1	491	0.389	0.348	0.255	514	454	506	472	0	5
		Cr2	531	0.450	0.400	0.295	552	492	544	510	3	5
Cobalt	Co 27	Co4	57	0.816	0.624	0.386	78	18	70	36	0	5
		Co3	658	0.118	0.118	0.091	673	613	665	631	0	15
		Co2	718	0.152	0.153	0.117	735	675	727	693	0	10
		Co1	777	0.323	0.322	0.243	798	738	790	756	3	5
Copper	Cu 29	Cu4	66	0.630	0.518	0.344	87	27	79	45	0	5
		Cu3	778	0.047	0.055	0.048	793	733	785	751	0	30
		Cu2	842	0.086	0.100	0.087	864.5	804.5	856.5	822.5	0	15
		Cu1	922	0.282	0.333	0.292	943.5	883.5	935.5	901.5	3	5
Dysprosium	Dy 66	Dy1	154	0.187	0.108	0.064	168.5	108.5	160.5	126.5	0	30
		Dy3	978	0.021	0.020	0.016	979	919	971	937	0	90
		Dy2	1127	0.028	0.026	0.022	1138	1078	1130	1096	3	70
		Dy4	1284	0.014	0.013	0.010	1299	1239	1291	1257	0	150
Erbium	Er 68	Er1	168	0.131	0.098	0.063	174	114	166	132	0	30
		Er3	1060	0.013	0.016	0.016	1065	1005	1057	1023	0	95
		Er2	1228	0.021	0.026	0.024	1236	1176	1228	1194	3	65
		Er4	1395	0.020	0.026	0.025	1411	1351	1403	1369	0	65
Europium	Eu 63	Eu1	107	0.403	0.273	0.176	130	70	122	88	0	10
		Eu3	140	0.222	0.150	0.096	162	102	154	120	0	20
		Eu2	860	0.040	0.039	0.035	869	809	861	827	3	40
		Eu4	988	0.041	0.039	0.035	999	939	991	957	0	45
Fluorine	F 9	F1	659	0.541	0.777	0.556	680	620	672	638	3	5

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

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### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )			Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	High	Low	High	Low			
Gadolinium Gd 64	Gd	Gd1	112	0.251	0.210	0.123	134	74	126	92	0	15
		Gd3	143	0.289	0.233	0.134	164.5	104.5	156.5	122.5	0	15
		Gd4	896	0.025	0.031	0.026	907	847	899	865	0	55
		Gd2	1030	0.026	0.034	0.029	1044	984	1036	1002	3	50
Gallium Ga 31	Ga	Ga4	58	0.303	0.231	0.137	80	20	72	38	0	15
		Ga3	974	0.069	0.080	0.066	996	936	988	954	0	25
		Ga1	1069	0.273	0.303	0.250	1091	1031	1083	1049	3	5
		Ga2	1096	0.145	0.153	0.128	1118	1058	1110	1076	0	10
Germanium Ge 32	Ge	Ge4	55	0.137	0.112	0.071	78	18	70	36	0	35
		Ge3	1047	0.042	0.051	0.044	1068.5	1008.5	1060.5	1026.5	0	35
		Ge1	1150	0.158	0.194	0.168	1171.5	1111.5	1163.5	1129.5	3	10
		Ge2	1181	0.072	0.090	0.078	1202	1142	1194	1160	0	20
Gold Au 79	Au	Au1	74	1.079	0.913	0.654	96	36	88	54	0	5
		Au2	243	0.064	0.059	0.044	264.5	204.5	256.5	222.5	0	40
		Au6	1522	0.004	0.008	0.010	1524	1464	1516	1482	0	175
		Au5	1771	0.008	0.016	0.018	1789	1729	1781	1747	0	90
		Au3	2022	0.022	0.045	0.054	2040	1980	2032	1998	3	25
		Au4	2107	0.011	0.031	0.039	2125	2065	2117	2083	0	35
Hafnium Hf 72	Hf	Hf1	184	0.192	0.167	0.103	195	135	187	153	0	20
		Hf4	1231	0.008	0.014	0.014	1241	1181	1233	1199	0	115
		Hf3	1427	0.017	0.029	0.028	1433	1373	1425	1391	0	60
		Hf2	1625	0.057	0.091	0.085	1644	1584	1636	1602	3	20
Holmium Ho 67	Ho	Ho1	162	0.145	0.114	0.067	175	115	167	133	0	30
		Ho3	1016	0.017	0.021	0.018	1020	960	1012	978	0	85
		Ho2	1177	0.028	0.035	0.030	1186	1126	1178	1144	3	50
		Ho4	1339	0.018	0.021	0.018	1354	1294	1346	1312	0	85
Indium In 49	In	In1	405	0.842	0.690	0.509	428	368	420	386	3	5
Iodine I 53	I	I1	510	0.302	0.287	0.322	531	471	523	489	3	5
		I2	519	0.301	0.271	0.286	541	481	533	499	0	5
		I3	562	0.035	0.041	0.041	584.5	524.5	576.5	542.5	0	35

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )			Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	High	Low	High	Low			
Iridium	Ir 77	Ir1	175	0.119	0.100	0.065	188	128	180	146	0	30
		Ir4	233	0.069	0.060	0.038	254	194	246	212	0	50
		Ir6	1439	0.005	0.011	0.011	1443	1383	1435	1401	0	145
		Ir5	1672	0.012	0.019	0.019	1690	1630	1682	1648	0	85
		Ir2	1909	0.031	0.061	0.064	1926	1866	1918	1884	3	25
		Ir3	1982	0.020	0.045	0.048	2000	1940	1992	1958	0	30
Iron	Fe 26	Fe4	50	1.209	0.929	0.572	73	13	65	31	0	5
		Fe1	600	0.158	0.152	0.113	616	556	608	574	3	15
		Fe2	654	0.230	0.222	0.163	672.5	612.5	664.5	630.5	0	10
		Fe3	705	0.275	0.265	0.192	727.5	667.5	719.5	685.5	0	10
Lanthanum	La 57	La1	83	0.656	0.457	0.283	105	45	97	63	0	10
		La2	634	0.087	0.082	0.064	644	584	636	602	3	25
		La3	732	0.029	0.027	0.020	736.5	676.5	728.5	694.5	0	70
Lead	Pb 82	Pb1	97	0.905	0.777	0.511	119	59	111	77	3	5
		Pb2	251	0.044	0.043	0.029	272	212	264	230	0	60
		Pb6	1641	-	0.004	0.005	1638	1578	1630	1596	0	340
		Pb5	1914	0.003	0.009	0.010	1910	1850	1902	1868	0	145
		Pb3	2188	0.005	0.020	0.022	2201	2141	2193	2159	0	60
		Pb4	2288	-	0.001	0.014	2303.5	2243.5	2295.5	2261.5	0	85
Lithium	Li 3	Li1	57	0.213	0.124	0.043	72	12	64	30	3	55
Lutetium	Lu 71	Lu1	182	0.154	0.124	0.075	194	134	186	152	0	25
		Lu4	1188	0.010	0.014	0.011	1198	1138	1190	1156	0	135
		Lu3	1378	0.017	0.024	0.020	1384	1324	1376	1342	0	75
		Lu2	1568	0.049	0.069	0.061	1586	1526	1578	1544	3	25
Magnesium	Mg 12	Mg1	48	0.691	0.513	0.315	71	11	63	29	0	10
		Mg2	1188	0.112	0.138	0.124	1199	1139	1191	1157	3	10

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )			Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	High	Low	High	Low			
Manganese	Mn 25	Mn4	45	0.927	0.673	0.412	67	7	59	25	0	5
		Mn1	545	0.210	0.192	0.135	561	501	553	519	3	10
		Mn2	592	0.270	0.243	0.177	611	551	603	569	0	10
		Mn3	638	0.205	0.184	0.134	660	600	652	618	0	10
Mercury	Hg 80	Hg1	81	0.877	0.723	0.486	103	43	95	61	3	5
		Hg2	246	0.049	0.043	0.031	268	208	260	226	0	60
		Hg5	1818	0.007	0.013	0.014	1836	1776	1828	1794	0	110
		Hg3	2078	0.019	0.030	0.034	2093	2033	2085	2051	0	40
		Hg4	2166	0.013	0.019	0.024	2184	2124	2176	2142	0	55
Molybdenum	Mo 42	Mo1	190	0.489	0.386	0.242	212	152	204	170	3	10
		Mo3	225	0.412	0.329	0.203	247	187	239	205	0	10
		Mo5	1881	0.004	0.009	0.011	1899	1839	1891	1857	0	145
		Mo2	2044	0.009	0.030	0.034	2062	2002	2054	2020	0	45
		Mo4	2149	0.003	0.013	0.015	2167	2107	2159	2125	0	90
Neodymium	Nd 60	Nd1	96	0.587	0.423	0.273	118	58	110	76	0	10
		Nd2	734	0.061	0.060	0.051	751	691	743	709	3	30
		Nd3	861	0.024	0.024	0.019	863	803	855	821	0	75
Nickel	Ni 28	Ni4	64	0.718	0.562	0.364	84	24	76	42	0	5
		Ni3	718	0.068	0.071	0.057	733	673	725	691	0	25
		Ni2	785	0.111	0.115	0.092	799	739	791	757	0	15
		Ni1	849	0.290	0.303	0.245	871	811	863	829	3	5
Niobium	Nb 41	Nb1	170	0.522	0.423	0.278	192.5	132.5	184.5	150.5	3	5
		Nb3	201	0.268	0.215	0.140	223.5	163.5	215.5	181.5	0	15
		Nb5	1787	0.005	0.012	0.013	1787	1727	1779	1745	0	125
		Nb2	1944	0.013	0.030	0.035	1962	1902	1954	1920	0	45
		Nb4	2039	0.008	0.013	0.016	2056	1996	2048	2014	0	90
Nitrogen	N 7	N1	389	0.389	0.293	0.191	407	347	399	365	3	10

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element		Region	Peak	Sensitivity Factor ( $S_x$ )			Acquisition		Analysis		*	†
				3 keV	5 keV	10 keV	High	Low	High	Low		
Osmium	Os 76	Os1	180	0.147	0.102	0.066	191	131	183	149	0	30
		Os4	226	0.061	0.042	0.027	247	187	239	205	0	65
		Os6	1396	0.007	0.010	0.010	1402	1342	1394	1360	0	160
		Os5	1622	0.012	0.017	0.017	1640	1580	1632	1598	0	95
		Os2	1850	0.044	0.064	0.065	1869	1809	1861	1827	3	25
		Os3	1920	0.028	0.043	0.044	1938	1878	1930	1896	0	35
Oxygen	O 8	O1	510	0.379	0.332	0.238	532	472	524	490	3	5
Palladium	Pd 46	Pd2	283	0.196	0.170	0.121	300	240	292	258	0	15
		Pd1	333	1.089	0.949	0.676	352.5	292.5	344.5	310.5	3	5
		Pd5	2282	-	0.004	0.004	2300	2240	2292	2258	0	270
Phosphorus	P 15	P1	123	1.300	0.962	0.582	145.5	85.5	137.5	103.5	3	5
		P2	1862	0.028	0.054	0.058	1880	1820	1872	1838	0	25
Platinum	Pt 78	Pt1	70	0.887	0.680	0.512	89	29	81	47	3	5
		Pt2	173	0.063	0.051	0.041	195	135	187	153	0	50
		Pt3	241	0.056	0.046	0.035	261.5	201.5	253.5	219.5	0	50
		Pt7	1484	0.004	0.008	0.010	1487	1427	1479	1445	0	175
		Pt6	1725	0.010	0.015	0.018	1743	1683	1735	1701	0	90
		Pt4	1969	0.025	0.047	0.057	1987	1927	1979	1945	3	25
		Pt5	2048	0.017	0.038	0.046	2067	2007	2059	2025	0	30
Potassium	K 19	K1	252	0.398	0.338	0.255	272	212	264	230	3	5
Praseodymium	Pr 59	Pr1	91	0.599	0.442	0.274	113.5	53.5	105.5	71.5	0	10
		Pr2	696	0.053	0.053	0.041	714	654	706	672	3	35
		Pr3	817	0.023	0.022	0.016	820	760	812	778	0	85
Rhenium	Re 75	Re1	179	0.224	0.182	0.116	188	128	180	146	0	15
		Re4	218	0.080	0.063	0.040	240	180	232	198	0	45
		Re6	1354	0.008	0.014	0.013	1361	1301	1353	1319	0	120
		Re5	1572	0.015	0.023	0.023	1590	1530	1582	1548	0	70
		Re2	1793	0.049	0.086	0.084	1812	1752	1804	1770	3	20
		Re3	1858	0.029	0.053	0.052	1877	1817	1869	1835	0	30

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )			Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	High	Low	High	Low			
Rhodium	Rh 45	Rh2	259	0.292	0.252	0.184	278	218	270	236	0	10
		Rh1	305	1.071	0.916	0.669	326	266	318	284	3	5
		Rh5	2180	–	0.004	0.006	2197	2137	2189	2155	0	230
		Rh3	2366	–	0.009	0.016	2381	2321	2373	2339	0	70
Rubidium	Rb 37	Rb5	78	0.090	0.068	0.049	98.5	38.5	90.5	56.5	0	45
		Rb4	107	0.040	0.029	0.021	128.5	68.5	120.5	86.5	0	105
		Rb3	1433	0.004	0.006	0.007	1438	1378	1430	1396	0	210
		Rb1	1561	0.015	0.021	0.027	1579	1519	1571	1537	3	60
		Rb2	1620	0.007	0.010	0.013	1639	1579	1631	1597	0	125
Ruthenium	Ru 44	Ru2	235	0.292	0.251	0.154	255	195	247	213	0	10
		Ru1	277	0.743	0.641	0.391	299	239	291	257	3	5
		Ru5	2078	–	0.006	0.006	2063	2003	2055	2021	0	210
		Ru3	2256	–	0.017	0.021	2273	2213	2265	2231	0	60
		Ru4	2385	–	0.007	0.009	2401	2341	2393	2359	0	120
Samarium	Sm 62	Sm1	103	0.348	0.260	0.169	125.5	65.5	117.5	83.5	0	15
		Sm3	135	0.168	0.120	0.072	145.5	85.5	137.5	103.5	0	30
		Sm2	814	0.039	0.041	0.033	826	766	818	784	3	45
		Sm4	940	0.028	0.030	0.024	952	892	944	910	0	60
Scandium	Sc 21	Sc1	343	0.374	0.307	0.206	362	302	354	320	3	10
		Sc2	370	0.388	0.318	0.212	393	333	385	351	0	10
Selenium	Se 34	Se5	47	0.049	0.040	0.044	69	9	61	27	2	55
		Se4	104	0.050	0.039	0.016	122	62	114	80	0	140
		Se3	1192	0.023	0.031	0.009	1213	1153	1205	1171	0	160
		Se1	1311	0.087	0.113	0.037	1331	1271	1323	1289	3	40
		Se2	1352	0.045	0.053	0.019	1372	1312	1364	1330	0	85
Silicon	Si 14	Si1	96	0.681	0.663	0.410	118	58	110	76	0	5
		Si3	96	0.260	0.227	0.189	118	58	110	76	0	5
		Si2	1621	0.041	0.084	0.087	1640	1580	1632	1598	3	20
		Si4	1621	0.077	0.123	0.147	1640	1580	1632	1598	0	20

\* Peak labeling (e.g., 0 = “none”).

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )			Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	High	Low	High	Low			
Silver	Ag 47	Ag1	359	1.212	1.064	0.769	376.5	316.5	368.5	334.5	3	5
		Ag4	2381	-	0.002	0.004	2399	2339	2391	2357	0	285
Sodium	Na 11	Na1	996	0.089	0.095	0.083	1011	951	1003	969	3	20
Strontium	Sr 38	Sr4	114	0.091	0.064	0.046	135	75	127	93	0	45
		Sr3	1516	0.006	0.007	0.008	1520	1460	1512	1478	0	190
		Sr1	1651	0.019	0.028	0.033	1665	1605	1657	1623	3	50
		Sr2	1718	0.008	0.011	0.013	1731	1671	1723	1689	0	125
Sulfur	S 16	S1	153	1.914	1.560	0.977	174.5	114.5	166.5	132.5	3	5
		S2	2119	0.013	0.024	0.031	2136	2076	2128	2094	0	45
Tantalum	Ta 73	Ta1	183	0.252	0.208	0.144	193	133	185	151	0	15
		Ta4	1271	0.009	0.014	0.015	1280	1220	1272	1238	0	100
		Ta3	1475	0.017	0.029	0.031	1479	1419	1471	1437	0	50
		Ta2	1680	0.056	0.091	0.097	1699	1639	1691	1657	3	15
Tellurium	Te 52	Te1	486	0.540	0.495	0.382	507	447	499	465	3	5
Terbium	Tb 65	Tb1	116	0.191	0.106	0.064	139	79	131	97	0	35
		Tb3	150	0.221	0.119	0.068	167	107	159	125	0	30
		Tb4	937	0.029	0.025	0.020	943	883	935	901	0	75
		Tb2	1078	0.033	0.030	0.023	1091	1031	1083	1049	3	65
		Tb5	1230	0.014	0.010	0.008	1247	1187	1239	1205	0	190
Thallium	Tl 81	Tl1	90	0.972	0.883	0.552	111.5	51.5	103.5	69.5	3	5
		Tl2	250	0.043	0.041	0.027	270	210	262	228	0	70
		Tl6	1601	-	0.005	0.005	1600	1540	1592	1558	0	330
		Tl5	1865	0.006	0.011	0.011	1863	1803	1855	1821	0	145
		Tl3	2132	0.009	0.024	0.025	2147	2087	2139	2105	0	55
		Tl4	2227	0.006	0.015	0.017	2243	2183	2235	2201	0	75
Thorium	Th 90	Th1	69	0.931	0.754	0.496	91.5	31.5	83.5	49.5	3	5
		Th2	249	0.092	0.088	0.065	271.5	211.5	263.5	229.5	0	25
		Th5	2296	-	0.002	0.003	2311	2251	2303	2269	0	420

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )			Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	High	Low	High	Low			
Thulium Tm 69	Tm	Tm1	170	0.174	0.124	0.083	179	119	171	137	3	25
		Tm4	1100	0.017	0.019	0.018	1108	1048	1100	1066	0	85
		Tm3	1278	0.026	0.028	0.028	1285	1225	1277	1243	0	55
		Tm2	1452	0.040	0.048	0.046	1469	1409	1461	1427	3	35
Tin Sn 50	Sn	Sn1	432	0.799	0.746	0.540	454	394	446	412	3	5
Titanium Ti 22	Ti	Ti1	390	0.387	0.326	0.223	408	348	400	366	0	5
		Ti2	421	0.605	0.511	0.346	444	384	436	402	3	5
Tungsten W 74	W	W1	182	0.252	0.203	0.131	193	133	185	151	0	15
		W5	210	0.050	0.039	0.026	232	172	224	190	0	70
		W4	1312	0.012	0.016	0.016	1320	1260	1312	1278	0	100
		W3	1524	0.021	0.029	0.028	1527	1467	1519	1485	0	60
		W2	1737	0.061	0.097	0.097	1755	1695	1747	1713	3	15
Uranium U 92	U	U1	77	1.515	1.116	0.771	99.5	39.5	91.5	57.5	3	5
		U2	284	0.246	0.214	0.170	307	247	299	265	0	10
Vanadium V 23	V	V1	440	0.325	0.286	0.203	457	397	449	415	0	10
		V2	475	0.506	0.440	0.310	497	437	489	455	3	5
Ytterbium Yb 70	Yb	Yb1	174	0.137	0.099	0.076	187	127	179	145	0	25
		Yb4	1141	0.010	0.012	0.014	1155	1095	1147	1113	0	115
		Yb3	1329	0.015	0.019	0.021	1334	1274	1326	1292	0	75
		Yb2	1511	0.040	0.051	0.056	1526	1466	1518	1484	3	30
Yttrium Y 39	Y	Y1	132	0.243	0.197	0.116	155.5	95.5	147.5	113.5	0	20
		Y4	1606	0.005	0.010	0.010	1608	1548	1600	1566	0	160
		Y2	1748	0.017	0.035	0.035	1764	1704	1756	1722	3	45
		Y3	1823	0.008	0.015	0.015	1840	1780	1832	1798	0	105

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )			Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	High	Low	High	Low			
Zinc	Zn 30	Zn4	64	0.574	0.457	0.320	86	26	78	44	0	5
		Zn3	839	0.040	0.044	0.041	853	793	845	811	0	35
		Zn2	908	0.085	0.095	0.090	930.5	870.5	922.5	888.5	0	15
		Zn1	997	0.282	0.325	0.305	1018	958	1010	976	3	5
Zirconium	Zr 40	Zr1	151	0.555	0.448	0.307	173.5	113.5	165.5	131.5	3	5
		Zr4	1695	0.009	0.015	0.018	1697	1637	1689	1655	0	90
		Zr2	1844	0.021	0.043	0.051	1861	1801	1853	1819	0	30
		Zr3	1929	0.007	0.018	0.023	1946	1886	1938	1904	0	65

Average matrix relative sensitivity factors for CMA

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

These values are valid only for data that have had a 5-point derivative applied to them.

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Aluminum	Al	Al1	70	0.285	0.266	0.159	0.118	0.096	0.081	0.071	92	32	84	50	0	10
		Al3	70	0.108	0.086	0.069	0.051	0.041	0.035	0.031	92	32	84	50	0	10
		Al2	1396	0.055	0.089	0.079	0.068	0.060	0.054	0.050	1416	1356	1408	1374	3	15
		Al4	1396	0.050	0.077	0.092	0.080	0.071	0.064	0.058	1416	1356	1408	1374	0	15
Antimony	Sb	Sb1	458	0.871	0.829	0.618	0.495	0.418	0.366	0.327	480	420	472	438	3	5
		Sb2	3035	-	0.004	0.008	0.009	0.009	0.008	0.008	3047	2987	3039	3005	0	185
Arsenic	As	As4	97	0.037	0.027	0.016	0.012	0.010	0.009	0.008	117.5	57.5	109.5	75.5	0	80
		As3	1118	0.061	0.066	0.029	0.025	0.022	0.019	0.018	1139.5	1079.5	1131.5	1097.5	0	45
		As1	1229	0.110	0.123	0.109	0.094	0.082	0.074	0.067	1250	1190	1242	1208	3	10
		As2	1264	0.051	0.058	0.053	0.045	0.040	0.036	0.033	1285	1225	1277	1243	0	25
Barium	Ba	Ba1	58	0.335	0.285	0.198	0.149	0.121	0.103	0.090	79	19	71	37	0	20
		Ba2	76	0.306	0.239	0.160	0.122	0.101	0.086	0.076	97	37	89	55	0	20
		Ba3	603	0.178	0.187	0.157	0.129	0.111	0.098	0.089	610.5	550.5	602.5	568.5	3	20
		Ba4	674	0.029	0.031	0.027	0.022	0.019	0.017	0.015	694	634	686	652	0	115
Beryllium	Be	Be1	108	0.130	0.092	0.053	0.040	0.032	0.028	0.024	128	68	120	86	3	10
Bismuth	Bi	Bi1	105	0.513	0.445	0.311	0.237	0.194	0.167	0.147	127	67	119	85	3	5
		Bi2	253	0.037	0.035	0.027	0.022	0.018	0.016	0.014	272	212	264	230	0	80
		Bi5	1960	-	0.011	0.013	0.012	0.011	0.010	0.010	1957	1897	1949	1915	0	200
		Bi3	2243	0.007	0.025	0.030	0.029	0.027	0.025	0.023	2256	2196	2248	2214	0	80
		Bi4	2350	-	0.020	0.022	0.021	0.019	0.018	0.017	2365	2305	2357	2323	0	110
Boron	B	B1	185	0.092	0.066	0.041	0.031	0.026	0.022	0.019	203	143	195	161	3	15
Bromine	Br	Br5	55	0.200	0.141	0.106	0.079	0.064	0.054	0.047	78	18	70	36	0	20
		Br4	102	0.096	0.076	0.057	0.043	0.036	0.030	0.027	126	66	118	84	0	35
		Br3	1267	0.031	0.037	0.038	0.033	0.029	0.026	0.024	1288	1228	1280	1246	0	45
		Br1	1393	0.090	0.118	0.129	0.112	0.099	0.090	0.082	1413.5	1353.5	1405.5	1371.5	3	15
		Br2	1439	0.056	0.063	0.071	0.062	0.055	0.050	0.046	1459.5	1399.5	1451.5	1417.5	0	25
Cadmium	Cd	Cd1	379	1.228	1.100	0.825	0.651	0.546	0.475	0.423	402	342	394	360	3	5
		Cd2	2694	-	0.007	0.013	0.014	0.013	0.012	0.012	2708	2648	2700	2666	0	125
Calcium	Ca	Ca1	297	0.445	0.357	0.238	0.186	0.155	0.134	0.120	314	254	306	272	3	10

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

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### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Carbon	C	C1	275	0.067	0.052	0.031	0.024	0.020	0.017	0.015	291	231	283	249	3	20
Cerium	Ce	Ce1	87	0.633	0.453	0.281	0.211	0.172	0.147	0.129	109.5	49.5	101.5	67.5	0	5
		Ce2	671	0.096	0.091	0.067	0.056	0.048	0.042	0.038	679	619	671	637	3	30
		Ce3	774	0.044	0.042	0.030	0.025	0.021	0.019	0.017	778	718	770	736	0	70
Cesium	Cs	Cs1	572	0.292	0.288	0.229	0.187	0.160	0.141	0.127	579	519	571	537	3	20
		Cs2	632	0.042	0.042	0.031	0.025	0.022	0.019	0.017	653	593	645	611	0	145
Chlorine	Cl	Cl1	184	2.784	1.907	1.513	1.157	0.952	0.817	0.722	206.5	146.5	198.5	164.5	3	5
Chromium	Cr	Cr1	491	0.240	0.216	0.159	0.128	0.108	0.095	0.085	514	454	506	472	0	5
		Cr2	531	0.282	0.252	0.186	0.150	0.127	0.111	0.099	552	492	544	510	3	5
Cobalt	Co	Co4	57	0.291	0.223	0.138	0.102	0.083	0.070	0.061	78	18	70	36	0	5
		Co3	658	0.077	0.077	0.059	0.049	0.042	0.037	0.033	673	613	665	631	0	15
		Co2	718	0.099	0.100	0.077	0.063	0.054	0.048	0.043	735	675	727	693	0	10
		Co1	777	0.211	0.211	0.160	0.131	0.112	0.099	0.089	798	738	790	756	3	5
Copper	Cu	Cu4	66	0.260	0.214	0.142	0.106	0.085	0.073	0.064	87	27	79	45	0	5
		Cu3	778	0.033	0.038	0.034	0.028	0.024	0.022	0.019	793	733	785	751	0	30
		Cu2	842	0.060	0.070	0.061	0.051	0.044	0.039	0.035	864.5	804.5	856.5	822.5	0	15
		Cu1	922	0.194	0.230	0.202	0.168	0.145	0.129	0.116	943.5	883.5	935.5	901.5	3	5
Dysprosium	Dy	Dy1	154	0.180	0.103	0.062	0.047	0.038	0.033	0.029	168.5	108.5	160.5	126.5	0	30
		Dy3	978	0.032	0.030	0.025	0.021	0.019	0.017	0.015	979	919	971	937	0	90
		Dy2	1127	0.042	0.038	0.033	0.029	0.025	0.023	0.021	1138	1078	1130	1096	3	70
		Dy4	1284	0.020	0.018	0.015	0.013	0.011	0.010	0.009	1299	1239	1291	1257	0	150
Erbium	Er	Er1	168	0.130	0.098	0.063	0.048	0.039	0.034	0.030	174	114	166	132	0	30
		Er3	1060	0.020	0.024	0.024	0.020	0.018	0.016	0.015	1065	1005	1057	1023	0	95
		Er2	1228	0.031	0.039	0.036	0.031	0.027	0.024	0.022	1236	1176	1228	1194	3	65
		Er4	1395	0.029	0.037	0.036	0.031	0.027	0.024	0.022	1411	1351	1403	1369	0	65
Europium	Eu	Eu1	107	0.476	0.321	0.207	0.157	0.128	0.110	0.096	130	70	122	88	0	10
		Eu3	140	0.279	0.188	0.121	0.091	0.075	0.064	0.056	162	102	154	120	0	20
		Eu2	860	0.077	0.075	0.066	0.056	0.049	0.044	0.040	869	809	861	827	3	40
		Eu4	988	0.078	0.075	0.067	0.056	0.049	0.044	0.040	999	939	991	957	0	45
Fluorine	F	F1	659	0.133	0.194	0.141	0.114	0.097	0.085	0.076	680	620	672	638	3	5

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Gadolinium	Gd	Gd1	112	0.222	0.185	0.109	0.082	0.067	0.058	0.051	134	74	126	92	0	15
		Gd3	143	0.277	0.222	0.128	0.097	0.079	0.068	0.060	164.5	104.5	156.5	122.5	0	15
		Gd4	896	0.039	0.049	0.040	0.034	0.030	0.027	0.024	907	847	899	865	0	55
		Gd2	1030	0.041	0.052	0.044	0.037	0.032	0.029	0.026	1044	984	1036	1002	3	50
Gallium	Ga	Ga4	58	0.088	0.067	0.040	0.030	0.024	0.021	0.018	80	20	72	38	0	15
		Ga3	974	0.037	0.043	0.036	0.030	0.026	0.023	0.021	996	936	988	954	0	25
		Ga1	1069	0.145	0.162	0.134	0.113	0.098	0.088	0.079	1091	1031	1083	1049	3	5
		Ga2	1096	0.076	0.081	0.069	0.058	0.050	0.045	0.041	1118	1058	1110	1076	0	10
Germanium	Ge	Ge4	55	0.067	0.055	0.035	0.026	0.022	0.018	0.016	78	18	70	36	0	35
		Ge3	1047	0.041	0.050	0.044	0.037	0.033	0.029	0.026	1068.5	1008.5	1060.5	1026.5	0	35
		Ge1	1150	0.152	0.188	0.163	0.139	0.121	0.108	0.099	1171.5	1111.5	1163.5	1129.5	3	10
		Ge2	1181	0.069	0.086	0.075	0.064	0.056	0.050	0.046	1202	1142	1194	1160	0	20
Gold	Au	Au1	74	0.509	0.430	0.307	0.229	0.186	0.158	0.139	96	36	88	54	0	5
		Au2	243	0.048	0.044	0.033	0.026	0.021	0.019	0.017	264.5	204.5	256.5	222.5	0	40
		Au6	1522	0.004	0.008	0.009	0.009	0.008	0.007	0.007	1524	1464	1516	1482	0	175
		Au5	1771	0.008	0.015	0.018	0.016	0.015	0.014	0.013	1789	1729	1781	1747	0	90
		Au3	2022	0.024	0.049	0.058	0.053	0.048	0.044	0.041	2040	1980	2032	1998	3	25
		Au4	2107	0.013	0.036	0.045	0.041	0.037	0.034	0.032	2125	2065	2117	2083	0	35
Hafnium	Hf	Hf1	184	0.107	0.093	0.057	0.044	0.037	0.031	0.028	195	135	187	153	0	20
		Hf4	1231	0.007	0.011	0.011	0.010	0.009	0.008	0.007	1241	1181	1233	1199	0	115
		Hf3	1427	0.013	0.023	0.022	0.019	0.017	0.015	0.014	1433	1373	1425	1391	0	60
		Hf2	1625	0.045	0.071	0.066	0.058	0.052	0.047	0.043	1644	1584	1636	1602	3	20
Holmium	Ho	Ho1	162	0.142	0.111	0.065	0.049	0.041	0.035	0.031	175	115	167	133	0	30
		Ho3	1016	0.025	0.032	0.027	0.023	0.020	0.018	0.017	1020	960	1012	978	0	85
		Ho2	1177	0.042	0.052	0.044	0.038	0.033	0.030	0.027	1186	1126	1178	1144	3	50
		Ho4	1339	0.025	0.030	0.025	0.022	0.019	0.017	0.016	1354	1294	1346	1312	0	85
Indium	In	In1	405	0.945	0.774	0.570	0.452	0.380	0.331	0.295	428	368	420	386	3	5
		In2	2806	-	0.005	0.009	0.010	0.009	0.009	0.008	2818	2758	2810	2776	0	180
Iodine	I	I1	510	0.404	0.385	0.432	0.349	0.296	0.260	0.233	531	471	523	489	3	5
		I2	519	0.404	0.364	0.385	0.311	0.265	0.232	0.209	541	481	533	499	0	5
		I3	562	0.048	0.056	0.056	0.045	0.038	0.033	0.030	584.5	524.5	576.5	542.5	0	35

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Iridium	Ir	Ir1	175	0.067	0.056	0.037	0.029	0.025	0.022	0.019	188	128	180	146	0	30
		Ir4	233	0.044	0.038	0.024	0.019	0.015	0.013	0.012	254	194	246	212	0	50
		Ir6	1439	0.004	0.009	0.009	0.008	0.008	0.007	0.006	1443	1383	1435	1401	0	145
		Ir5	1672	0.011	0.017	0.017	0.015	0.014	0.013	0.012	1690	1630	1682	1648	0	85
		Ir2	1909	0.028	0.055	0.057	0.052	0.047	0.043	0.040	1926	1866	1918	1884	3	25
		Ir3	1982	0.019	0.042	0.044	0.041	0.037	0.034	0.031	2000	1940	1992	1958	0	30
Iron	Fe	Fe4	50	0.416	0.320	0.197	0.146	0.118	0.100	0.087	73	13	65	31	0	5
		Fe1	600	0.102	0.099	0.074	0.060	0.051	0.045	0.041	616	556	608	574	3	15
		Fe2	654	0.151	0.146	0.107	0.087	0.075	0.066	0.059	672.5	612.5	664.5	630.5	0	10
		Fe3	705	0.181	0.176	0.127	0.104	0.089	0.078	0.070	727.5	667.5	719.5	685.5	0	10
Lanthanum	La	La1	83	0.598	0.416	0.257	0.198	0.163	0.140	0.124	105	45	97	63	0	10
		La2	634	0.129	0.120	0.094	0.078	0.067	0.059	0.054	644	584	636	602	3	25
		La3	732	0.044	0.040	0.031	0.025	0.022	0.019	0.017	736.5	676.5	728.5	694.5	0	70
Lead	Pb	Pb1	97	0.712	0.610	0.400	0.303	0.248	0.213	0.187	119	59	111	77	3	5
		Pb2	251	0.048	0.046	0.032	0.025	0.021	0.018	0.016	272	212	264	230	0	60
		Pb6	1641	-	0.005	0.007	0.006	0.006	0.005	0.005	1638	1578	1630	1596	0	340
		Pb5	1914	0.005	0.013	0.015	0.014	0.013	0.012	0.011	1910	1850	1902	1868	0	145
		Pb3	2188	0.008	0.033	0.038	0.035	0.033	0.030	0.028	2201	2141	2193	2159	0	60
		Pb4	2288	-	0.002	0.026	0.025	0.023	0.021	0.020	2303.5	2243.5	2295.5	2261.5	0	85
Lithium	Li	Li1	57	0.026	0.015	0.005	0.004	0.003	0.003	0.002	72	12	64	30	3	55
Lutetium	Lu	Lu1	182	0.161	0.129	0.078	0.060	0.049	0.042	0.037	194	134	186	152	0	25
		Lu4	1188	0.016	0.021	0.017	0.015	0.014	0.012	0.011	1198	1138	1190	1156	0	135
		Lu3	1378	0.025	0.035	0.030	0.026	0.023	0.021	0.019	1384	1324	1376	1342	0	75
		Lu2	1568	0.070	0.100	0.087	0.076	0.068	0.062	0.056	1586	1526	1578	1544	3	25
Magnesium	Mg	Mg1	48	0.526	0.392	0.242	0.178	0.144	0.122	0.106	71	11	63	29	0	10
		Mg2	1188	0.084	0.105	0.096	0.081	0.071	0.064	0.058	1199	1139	1191	1157	3	10
Manganese	Mn	Mn4	45	0.322	0.234	0.143	0.106	0.085	0.072	0.063	67	7	59	25	0	5
		Mn1	545	0.136	0.125	0.088	0.071	0.061	0.053	0.048	561	501	553	519	3	10
		Mn2	592	0.177	0.160	0.117	0.094	0.080	0.070	0.063	611	551	603	569	0	10
		Mn3	638	0.136	0.122	0.089	0.072	0.061	0.054	0.048	660	600	652	618	0	10

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Mercury	Hg	Hg1	81	0.657	0.541	0.363	0.273	0.222	0.189	0.166	103	43	95	61	3	5
		Hg2	246	0.051	0.044	0.032	0.025	0.021	0.018	0.016	268	208	260	226	0	60
		Hg5	1818	0.009	0.017	0.018	0.017	0.015	0.014	0.013	1836	1776	1828	1794	0	110
		Hg3	2078	0.027	0.042	0.048	0.044	0.040	0.037	0.034	2093	2033	2085	2051	0	40
		Hg4	2166	0.020	0.028	0.036	0.033	0.031	0.028	0.026	2184	2124	2176	2142	0	55
Molybdenum	Mo	Mo1	190	0.273	0.216	0.135	0.104	0.086	0.074	0.065	212	152	204	170	3	10
		Mo3	225	0.244	0.195	0.120	0.093	0.076	0.066	0.058	247	187	239	205	0	10
		Mo5	1881	0.003	0.007	0.008	0.007	0.007	0.006	0.006	1899	1839	1891	1857	0	145
		Mo2	2044	0.007	0.024	0.027	0.025	0.023	0.021	0.020	2062	2002	2054	2020	0	45
		Mo4	2149	0.003	0.011	0.013	0.012	0.011	0.010	0.010	2167	2107	2159	2125	0	90
Neodymium	Nd	Nd1	96	0.521	0.375	0.242	0.182	0.149	0.127	0.112	118	58	110	76	0	10
		Nd2	734	0.094	0.092	0.077	0.064	0.056	0.049	0.045	751	691	743	709	3	30
		Nd3	861	0.036	0.036	0.029	0.024	0.021	0.019	0.017	863	803	855	821	0	75
Nickel	Ni	Ni4	64	0.277	0.217	0.141	0.104	0.084	0.072	0.063	84	24	76	42	0	5
		Ni3	718	0.044	0.046	0.037	0.031	0.026	0.023	0.021	733	673	725	691	0	25
		Ni2	785	0.071	0.074	0.060	0.049	0.043	0.038	0.034	799	739	791	757	0	15
		Ni1	849	0.187	0.195	0.158	0.131	0.112	0.099	0.090	871	811	863	829	3	5
Niobium	Nb	Nb1	170	0.303	0.245	0.161	0.123	0.102	0.088	0.077	192.5	132.5	184.5	150.5	3	5
		Nb3	201	0.164	0.131	0.086	0.066	0.054	0.047	0.041	223.5	163.5	215.5	181.5	0	15
		Nb5	1787	0.004	0.009	0.010	0.009	0.008	0.008	0.007	1787	1727	1779	1745	0	125
		Nb2	1944	0.010	0.023	0.028	0.026	0.024	0.022	0.020	1962	1902	1954	1920	0	45
		Nb4	2039	0.006	0.011	0.013	0.013	0.012	0.011	0.010	2056	1996	2048	2014	0	90
Nitrogen	N	N1	389	0.191	0.144	0.095	0.075	0.062	0.054	0.048	407	347	399	365	3	10
Osmium	Os	Os1	180	0.079	0.055	0.035	0.028	0.023	0.020	0.018	191	131	183	149	0	30
		Os4	226	0.036	0.025	0.016	0.012	0.010	0.009	0.008	247	187	239	205	0	65
		Os6	1396	0.006	0.008	0.008	0.007	0.006	0.006	0.005	1402	1342	1394	1360	0	160
		Os5	1622	0.010	0.014	0.014	0.012	0.011	0.010	0.009	1640	1580	1632	1598	0	95
		Os2	1850	0.037	0.053	0.054	0.049	0.044	0.040	0.037	1869	1809	1861	1827	3	25
		Os3	1920	0.024	0.036	0.037	0.034	0.031	0.028	0.026	1938	1878	1930	1896	0	35
Oxygen	O	O1	510	0.152	0.135	0.097	0.078	0.065	0.057	0.051	532	472	524	490	3	5

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Palladium	Pd	Pd2	283	0.140	0.122	0.087	0.068	0.056	0.049	0.044	300	240	292	258	0	15
		Pd1	333	0.823	0.717	0.510	0.399	0.333	0.288	0.256	352.5	292.5	344.5	310.5	3	5
		Pd5	2282	-	0.004	0.005	0.005	0.005	0.004	0.004	2300	2240	2292	2258	0	270
		Pd3	2476	-	0.012	0.016	0.016	0.015	0.014	0.014	2492	2432	2484	2450	0	75
		Pd4	2633	-	0.005	0.008	0.008	0.007	0.007	0.006	2650	2590	2642	2608	0	160
Phosphorus	P	P1	123	0.802	0.595	0.361	0.272	0.223	0.190	0.167	145.5	85.5	137.5	103.5	3	5
		P2	1862	0.023	0.044	0.047	0.043	0.039	0.036	0.033	1880	1820	1872	1838	0	25
Platinum	Pt	Pt1	70	0.361	0.276	0.208	0.155	0.125	0.106	0.093	89	29	81	47	3	5
		Pt2	173	0.038	0.031	0.025	0.019	0.016	0.014	0.012	195	135	187	153	0	50
		Pt3	241	0.039	0.031	0.024	0.019	0.016	0.013	0.012	261.5	201.5	253.5	219.5	0	50
		Pt7	1484	0.003	0.008	0.009	0.008	0.007	0.007	0.006	1487	1427	1479	1445	0	175
		Pt6	1725	0.009	0.013	0.017	0.015	0.014	0.013	0.012	1743	1683	1735	1701	0	90
		Pt4	1969	0.025	0.047	0.056	0.052	0.047	0.043	0.040	1987	1927	1979	1945	3	25
		Pt5	2048	0.018	0.039	0.047	0.044	0.040	0.037	0.034	2067	2007	2059	2025	0	30
Potassium	K	K1	252	0.874	0.746	0.563	0.437	0.363	0.314	0.278	272	212	264	230	3	5
Praseodymium	Pr	Pr1	91	0.525	0.387	0.240	0.180	0.147	0.126	0.110	113.5	53.5	105.5	71.5	0	10
		Pr2	696	0.079	0.079	0.061	0.051	0.044	0.039	0.035	714	654	706	672	3	35
		Pr3	817	0.034	0.032	0.024	0.020	0.017	0.015	0.014	820	760	812	778	0	85
Rhenium	Re	Re1	179	0.115	0.093	0.059	0.046	0.038	0.033	0.029	188	128	180	146	0	15
		Re4	218	0.044	0.035	0.022	0.017	0.014	0.012	0.011	240	180	232	198	0	45
		Re6	1354	0.007	0.011	0.010	0.009	0.008	0.008	0.007	1361	1301	1353	1319	0	120
		Re5	1572	0.011	0.018	0.018	0.016	0.014	0.013	0.012	1590	1530	1582	1548	0	70
		Re2	1793	0.039	0.067	0.065	0.059	0.053	0.048	0.044	1812	1752	1804	1770	3	20
		Re3	1858	0.024	0.042	0.041	0.037	0.033	0.030	0.028	1877	1817	1869	1835	0	30
Rhodium	Rh	Rh2	259	0.187	0.161	0.118	0.092	0.076	0.066	0.059	278	218	270	236	0	10
		Rh1	305	0.725	0.620	0.453	0.353	0.293	0.254	0.226	326	266	318	284	3	5
		Rh5	2180	-	0.004	0.005	0.005	0.005	0.005	0.004	2197	2137	2189	2155	0	230
		Rh3	2366	-	0.010	0.017	0.017	0.016	0.015	0.014	2381	2321	2373	2339	0	70
		Rh4	2507	-	0.005	0.009	0.009	0.008	0.008	0.007	2525	2465	2517	2483	0	135

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Rubidium	Rb	Rb5	78	0.197	0.149	0.108	0.081	0.066	0.056	0.050	98.5	38.5	90.5	56.5	0	45
		Rb4	107	0.088	0.063	0.046	0.035	0.029	0.025	0.022	128.5	68.5	120.5	86.5	0	105
		Rb3	1433	0.009	0.015	0.018	0.016	0.014	0.013	0.012	1438	1378	1430	1396	0	210
		Rb1	1561	0.036	0.051	0.066	0.059	0.053	0.048	0.044	1579	1519	1571	1537	3	60
		Rb2	1620	0.018	0.024	0.033	0.030	0.027	0.024	0.022	1639	1579	1631	1597	0	125
Ruthenium	Ru	Ru2	235	0.175	0.151	0.092	0.072	0.060	0.051	0.046	255	195	247	213	0	10
		Ru1	277	0.473	0.407	0.249	0.193	0.160	0.138	0.123	299	239	291	257	3	5
		Ru5	2078	-	0.005	0.005	0.005	0.005	0.004	0.004	2063	2003	2055	2021	0	210
		Ru3	2256	-	0.017	0.020	0.019	0.018	0.017	0.016	2273	2213	2265	2231	0	60
		Ru4	2385	-	0.008	0.010	0.009	0.009	0.008	0.008	2401	2341	2393	2359	0	120
Samarium	Sm	Sm1	103	0.305	0.228	0.148	0.112	0.091	0.078	0.069	125.5	65.5	117.5	83.5	0	15
		Sm3	135	0.160	0.114	0.069	0.053	0.044	0.038	0.034	145.5	85.5	137.5	103.5	0	30
		Sm2	814	0.060	0.063	0.051	0.043	0.037	0.033	0.030	826	766	818	784	3	45
		Sm4	940	0.043	0.046	0.036	0.031	0.027	0.024	0.022	952	892	944	910	0	60
Scandium	Sc	Sc1	343	0.308	0.254	0.171	0.135	0.113	0.098	0.087	362	302	354	320	3	10
		Sc2	370	0.324	0.267	0.179	0.141	0.118	0.102	0.091	393	333	385	351	0	10
Selenium	Se	Se5	47	0.031	0.025	0.028	0.020	0.017	0.014	0.012	69	9	61	27	2	55
		Se4	104	0.036	0.028	0.012	0.009	0.007	0.006	0.006	122	62	114	80	0	140
		Se3	1192	0.024	0.032	0.009	0.008	0.007	0.006	0.006	1213	1153	1205	1171	0	160
		Se1	1311	0.087	0.114	0.038	0.033	0.029	0.026	0.024	1331	1271	1323	1289	3	40
		Se2	1352	0.045	0.053	0.019	0.016	0.014	0.013	0.012	1372	1312	1364	1330	0	85
Silicon	Si	Si1	96	0.424	0.414	0.257	0.192	0.156	0.133	0.117	118	58	110	76	0	5
		Si3	96	0.071	0.063	0.053	0.040	0.032	0.027	0.024	118	58	110	76	0	5
		Si2	1621	0.029	0.060	0.063	0.056	0.050	0.045	0.041	1640	1580	1632	1598	3	20
		Si4	1621	0.028	0.046	0.056	0.049	0.044	0.040	0.037	1640	1580	1632	1598	0	20

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Silver	Ag	Ag1	359	1.000	0.877	0.633	0.497	0.416	0.361	0.321	376.5	316.5	368.5	334.5	3	5
		Ag4	2381	-	0.003	0.005	0.005	0.005	0.005	0.004	2399	2339	2391	2357	0	285
		Ag2	2583	-	0.008	0.016	0.016	0.015	0.014	0.013	2598	2538	2590	2556	0	90
		Ag3	2755	-	0.003	0.007	0.007	0.007	0.007	0.006	2771	2711	2763	2729	0	200
Sodium	Na	Na1	996	0.081	0.088	0.078	0.065	0.056	0.050	0.045	1011	951	1003	969	3	20
Strontium	Sr	Sr4	114	0.124	0.087	0.063	0.049	0.041	0.035	0.031	135	75	127	93	0	45
		Sr3	1516	0.010	0.012	0.014	0.013	0.012	0.010	0.010	1520	1460	1512	1478	0	190
		Sr1	1651	0.032	0.047	0.055	0.049	0.044	0.040	0.037	1665	1605	1657	1623	3	50
		Sr2	1718	0.014	0.018	0.022	0.020	0.018	0.017	0.015	1731	1671	1723	1689	0	125
Sulfur	S	S1	153	1.454	1.186	0.743	0.565	0.464	0.398	0.351	174.5	114.5	166.5	132.5	3	5
		S2	2119	0.015	0.027	0.035	0.033	0.030	0.028	0.026	2136	2076	2128	2094	0	45
Tantalum	Ta	Ta1	183	0.131	0.108	0.074	0.057	0.047	0.041	0.036	193	133	185	151	0	15
		Ta4	1271	0.007	0.011	0.012	0.010	0.009	0.008	0.008	1280	1220	1272	1238	0	100
		Ta3	1475	0.013	0.022	0.023	0.021	0.019	0.017	0.016	1479	1419	1471	1437	0	50
		Ta2	1680	0.042	0.068	0.072	0.064	0.057	0.052	0.048	1699	1639	1691	1657	3	15
Tellurium	Te	Te1	486	0.637	0.582	0.448	0.361	0.306	0.268	0.240	507	447	499	465	3	5
Terbium	Tb	Tb1	116	0.168	0.093	0.056	0.042	0.035	0.030	0.026	139	79	131	97	0	35
		Tb3	150	0.212	0.114	0.065	0.049	0.040	0.034	0.030	167	107	159	125	0	30
		Tb4	937	0.045	0.038	0.030	0.025	0.022	0.020	0.018	943	883	935	901	0	75
		Tb2	1078	0.050	0.045	0.035	0.030	0.026	0.023	0.021	1091	1031	1083	1049	3	65
		Tb5	1230	0.020	0.015	0.012	0.010	0.009	0.008	0.007	1247	1187	1239	1205	0	190
Thallium	Tl	Tl1	90	0.706	0.641	0.400	0.302	0.246	0.211	0.185	111.5	51.5	103.5	69.5	3	5
		Tl2	250	0.044	0.043	0.027	0.022	0.018	0.016	0.014	270	210	262	228	0	70
		Tl6	1601	-	0.006	0.006	0.006	0.005	0.005	0.005	1600	1540	1592	1558	0	330
		Tl5	1865	0.008	0.014	0.014	0.013	0.012	0.011	0.010	1863	1803	1855	1821	0	145
		Tl3	2132	0.014	0.038	0.039	0.037	0.033	0.031	0.029	2147	2087	2139	2105	0	55
		Tl4	2227	0.010	0.025	0.028	0.026	0.024	0.022	0.021	2243	2183	2235	2201	0	75

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

These sensitivity factors may not be distributed without written permission from Physical Electronics, Inc.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Thorium	Th	Th1	69	0.505	0.407	0.267	0.209	0.175	0.152	0.135	91.5	31.5	83.5	49.5	3	5
		Th2	249	0.069	0.066	0.049	0.040	0.034	0.030	0.027	271.5	211.5	263.5	229.5	0	25
		Th5	2296	-	0.002	0.003	0.003	0.003	0.003	0.003	2311	2251	2303	2269	0	420
		Th3	2634	-	0.006	0.008	0.008	0.007	0.007	0.007	2645	2585	2637	2603	0	200
		Th4	2789	-	0.003	0.005	0.006	0.005	0.005	0.005	2803	2743	2795	2761	0	280
Thulium	Tm	Tm1	170	0.166	0.118	0.079	0.060	0.050	0.043	0.038	179	119	171	137	3	25
		Tm4	1100	0.025	0.028	0.026	0.023	0.020	0.018	0.016	1108	1048	1100	1066	0	85
		Tm3	1278	0.036	0.039	0.039	0.034	0.030	0.027	0.025	1285	1225	1277	1243	0	55
		Tm2	1452	0.054	0.065	0.062	0.054	0.047	0.043	0.039	1469	1409	1461	1427	3	35
Tin	Sn	Sn1	432	0.942	0.879	0.635	0.506	0.427	0.373	0.333	454	394	446	412	3	5
		Sn2	2919	0.000	0.004	0.008	0.009	0.009	0.008	0.008	2933	2873	2925	2891	0	215
Titanium	Ti	Ti1	390	0.275	0.232	0.160	0.127	0.106	0.093	0.083	408	348	400	366	0	5
		Ti2	421	0.437	0.370	0.251	0.199	0.167	0.146	0.130	444	384	436	402	3	5
Tungsten	W	W1	182	0.129	0.104	0.067	0.052	0.043	0.037	0.033	193	133	185	151	0	15
		W5	210	0.027	0.021	0.014	0.011	0.009	0.008	0.007	232	172	224	190	0	70
		W4	1312	0.009	0.013	0.013	0.011	0.010	0.009	0.009	1320	1260	1312	1278	0	100
		W3	1524	0.016	0.022	0.021	0.019	0.017	0.015	0.014	1527	1467	1519	1485	0	60
		W2	1737	0.046	0.073	0.073	0.065	0.059	0.053	0.049	1755	1695	1747	1713	3	15
Uranium	U	U1	77	0.607	0.446	0.307	0.242	0.202	0.176	0.157	99.5	39.5	91.5	57.5	3	5
		U2	284	0.169	0.146	0.116	0.095	0.082	0.072	0.065	307	247	299	265	0	10
		U5	2414	-	0.003	0.004	0.004	0.004	0.004	0.004	2429	2369	2421	2387	0	330
		U3	2764	-	0.004	0.008	0.008	0.008	0.008	0.007	2780	2720	2772	2738	0	165
		U4	2940	-	0.004	0.007	0.007	0.007	0.007	0.006	2955	2895	2947	2913	0	200
Vanadium	V	V1	440	0.211	0.186	0.133	0.106	0.090	0.078	0.070	457	397	449	415	0	10
		V2	475	0.334	0.292	0.206	0.164	0.138	0.121	0.108	497	437	489	455	3	5
Ytterbium	Yb	Yb1	174	0.176	0.127	0.097	0.074	0.061	0.052	0.046	187	127	179	145	0	25
		Yb4	1141	0.019	0.024	0.026	0.022	0.020	0.018	0.016	1155	1095	1147	1113	0	115
		Yb3	1329	0.028	0.034	0.038	0.034	0.030	0.027	0.025	1334	1274	1326	1292	0	75
		Yb2	1511	0.071	0.090	0.098	0.086	0.076	0.069	0.063	1526	1466	1518	1484	3	30
Yttrium	Y	Y1	132	0.221	0.179	0.106	0.082	0.068	0.059	0.053	155.5	95.5	147.5	113.5	0	20
		Y4	1606	0.006	0.012	0.012	0.011	0.010	0.009	0.008	1608	1548	1600	1566	0	160
		Y2	1748	0.020	0.042	0.042	0.038	0.035	0.032	0.029	1764	1704	1756	1722	3	45
		Y3	1823	0.010	0.019	0.019	0.017	0.016	0.014	0.013	1840	1780	1832	1798	0	105
Zinc	Zn	Zn4	64	0.242	0.193	0.135	0.101	0.082	0.070	0.061	86	26	78	44	0	5
		Zn3	839	0.032	0.035	0.033	0.027	0.024	0.021	0.019	853	793	845	811	0	35
		Zn2	908	0.067	0.075	0.071	0.060	0.052	0.046	0.042	930.5	870.5	922.5	888.5	0	15
		Zn1	997	0.220	0.254	0.239	0.200	0.173	0.154	0.140	1018	958	1010	976	3	5

\* Peak labeling (e.g., 0 = "none").

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Zirconium	Zr	Zr1	151	0.405	0.327	0.224	0.175	0.146	0.127	0.113	173.5	113.5	165.5	131.5	3	5
		Zr4	1695	0.008	0.014	0.018	0.016	0.015	0.014	0.013	1697	1637	1689	1655	0	90
		Zr2	1844	0.021	0.043	0.051	0.047	0.043	0.039	0.036	1861	1801	1853	1819	0	30
		Zr3	1929	0.007	0.019	0.024	0.022	0.020	0.018	0.017	1946	1886	1938	1904	0	65

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

#### Average matrix relative sensitivity factors for SCA

These values are valid only for data that have had a 5-point derivative applied to them.

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Aluminum	Al	Al1	70	0.493	0.460	0.275	0.204	0.166	0.140	0.123	92	32	84	50	0	10
		Al3	70	0.187	0.149	0.119	0.088	0.071	0.061	0.054	92	32	84	50	0	10
		Al2	1396	0.065	0.106	0.094	0.081	0.071	0.064	0.059	1416	1356	1408	1374	3	15
		Al4	1396	0.059	0.092	0.109	0.095	0.084	0.076	0.069	1416	1356	1408	1374	0	15
Antimony	Sb	Sb1	458	0.999	0.950	0.708	0.567	0.479	0.420	0.375	480	420	472	438	3	5
Arsenic	As	As4	97	0.061	0.044	0.026	0.020	0.016	0.015	0.013	117.5	57.5	109.5	75.5	0	80
		As3	1118	0.068	0.074	0.033	0.028	0.025	0.021	0.020	1139.5	1079.5	1131.5	1097.5	0	45
		As1	1229	0.126	0.141	0.125	0.108	0.094	0.085	0.077	1250	1190	1242	1208	3	10
		As2	1264	0.059	0.067	0.061	0.052	0.046	0.042	0.038	1285	1225	1277	1243	0	25
Barium	Ba	Ba1	58	0.594	0.505	0.351	0.264	0.215	0.183	0.160	79	19	71	37	0	20
		Ba2	76	0.523	0.408	0.273	0.209	0.173	0.147	0.130	97	37	89	55	0	20
		Ba3	603	0.195	0.205	0.172	0.141	0.121	0.107	0.097	610.5	550.5	602.5	568.5	3	20
		Ba4	674	0.031	0.034	0.029	0.024	0.021	0.018	0.016	694	634	686	652	0	115
Beryllium	Be	Be1	108	0.209	0.148	0.085	0.064	0.052	0.045	0.039	128	68	120	86	3	10
Bismuth	Bi	Bi1	105	0.831	0.720	0.503	0.384	0.314	0.270	0.238	127	67	119	85	3	5
		Bi2	253	0.049	0.046	0.036	0.029	0.024	0.021	0.019	272	212	264	230	0	80
		Bi5	1960	-	0.012	0.015	0.014	0.012	0.011	0.011	1957	1897	1949	1915	0	200
		Bi3	2243	0.007	0.023	0.028	0.027	0.025	0.023	0.021	2256	2196	2248	2214	0	80
		Bi4	2350	-	0.017	0.018	0.018	0.016	0.015	0.014	2365	2305	2357	2323	0	110
Boron	B	B1	185	0.132	0.095	0.059	0.044	0.037	0.032	0.027	203	143	195	161	3	15
Bromine	Br	Br5	55	0.357	0.252	0.189	0.141	0.114	0.096	0.084	78	18	70	36	0	20
		Br4	102	0.156	0.124	0.093	0.070	0.059	0.049	0.044	126	66	118	84	0	35
		Br3	1267	0.036	0.043	0.044	0.038	0.034	0.030	0.028	1288	1228	1280	1246	0	45
		Br1	1393	0.107	0.140	0.153	0.133	0.118	0.107	0.098	1413.5	1353.5	1405.5	1371.5	3	15
		Br2	1439	0.067	0.076	0.085	0.074	0.066	0.060	0.055	1459.5	1399.5	1451.5	1417.5	0	25
Cadmium	Cd	Cd1	379	1.469	1.316	0.987	0.779	0.653	0.568	0.506	402	342	394	360	3	5
Calcium	Ca	Ca1	297	0.566	0.454	0.303	0.237	0.197	0.170	0.153	314	254	306	272	3	10

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Carbon	C	C1	275	0.087	0.067	0.040	0.031	0.026	0.022	0.019	291	231	283	249	3	20
Cerium	Ce	Ce1	87	1.059	0.758	0.470	0.353	0.288	0.246	0.216	109.5	49.5	101.5	67.5	0	5
		Ce2	671	0.104	0.098	0.072	0.061	0.052	0.045	0.041	679	619	671	637	3	30
		Ce3	774	0.047	0.045	0.032	0.027	0.023	0.020	0.018	778	718	770	736	0	70
Cesium	Cs	Cs1	572	0.322	0.317	0.252	0.206	0.176	0.155	0.140	579	519	571	537	3	20
		Cs2	632	0.046	0.046	0.034	0.027	0.024	0.021	0.018	653	593	645	611	0	145
Chlorine	Cl	Cl1	184	3.996	2.737	2.172	1.661	1.367	1.173	1.036	206.5	146.5	198.5	164.5	3	5
Chromium	Cr	Cr1	491	0.271	0.244	0.180	0.145	0.122	0.107	0.096	514	454	506	472	0	5
		Cr2	531	0.314	0.281	0.207	0.167	0.142	0.124	0.110	552	492	544	510	3	5
Cobalt	Co	Co4	57	0.517	0.396	0.245	0.181	0.148	0.124	0.108	78	18	70	36	0	5
		Co3	658	0.083	0.083	0.064	0.053	0.046	0.040	0.036	673	613	665	631	0	15
		Co2	718	0.107	0.108	0.083	0.068	0.058	0.052	0.046	735	675	727	693	0	10
		Co1	777	0.227	0.227	0.172	0.141	0.120	0.106	0.096	798	738	790	756	3	5
Copper	Cu	Cu4	66	0.453	0.373	0.248	0.185	0.148	0.127	0.112	87	27	79	45	0	5
		Cu3	778	0.035	0.041	0.037	0.030	0.026	0.024	0.020	793	733	785	751	0	30
		Cu2	842	0.065	0.075	0.066	0.055	0.047	0.042	0.038	864.5	804.5	856.5	822.5	0	15
		Cu1	922	0.211	0.250	0.219	0.182	0.157	0.140	0.126	943.5	883.5	935.5	901.5	3	5
Dysprosium	Dy	Dy1	154	0.269	0.154	0.093	0.070	0.057	0.049	0.043	168.5	108.5	160.5	126.5	0	30
		Dy3	978	0.035	0.033	0.027	0.023	0.021	0.019	0.016	979	919	971	937	0	90
		Dy2	1127	0.047	0.043	0.037	0.033	0.028	0.026	0.024	1138	1078	1130	1096	3	70
		Dy4	1284	0.023	0.021	0.017	0.015	0.013	0.012	0.010	1299	1239	1291	1257	0	150
Erbium	Er	Er1	168	0.191	0.144	0.092	0.070	0.057	0.050	0.044	174	114	166	132	0	30
		Er3	1060	0.022	0.027	0.027	0.022	0.020	0.018	0.017	1065	1005	1057	1023	0	95
		Er2	1228	0.036	0.045	0.041	0.036	0.031	0.028	0.025	1236	1176	1228	1194	3	65
		Er4	1395	0.034	0.044	0.043	0.037	0.032	0.029	0.026	1411	1351	1403	1369	0	65
Erbium	Eu	Eu1	107	0.768	0.518	0.334	0.253	0.206	0.177	0.155	130	70	122	88	0	10
		Eu3	140	0.426	0.287	0.185	0.139	0.115	0.098	0.086	162	102	154	120	0	20
		Eu2	860	0.083	0.081	0.071	0.060	0.053	0.047	0.043	869	809	861	827	3	40
		Eu4	988	0.085	0.082	0.073	0.061	0.054	0.048	0.044	999	939	991	957	0	45
Fluorine	F	F1	659	0.144	0.210	0.153	0.124	0.105	0.092	0.082	680	620	672	638	3	5

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Gadolinium	Gd	Gd1	112	0.355	0.296	0.174	0.131	0.107	0.093	0.082	134	74	126	92	0	15
		Gd3	143	0.421	0.338	0.195	0.148	0.120	0.103	0.091	164.5	104.5	156.5	122.5	0	15
		Gd4	896	0.042	0.053	0.043	0.037	0.032	0.029	0.026	907	847	899	865	0	55
		Gd2	1030	0.045	0.057	0.049	0.041	0.035	0.032	0.029	1044	984	1036	1002	3	50
Gallium	Ga	Ga4	58	0.156	0.119	0.071	0.053	0.043	0.037	0.032	80	20	72	38	0	15
		Ga3	974	0.040	0.047	0.039	0.033	0.028	0.025	0.023	996	936	988	954	0	25
		Ga1	1069	0.161	0.180	0.149	0.126	0.109	0.098	0.088	1091	1031	1083	1049	3	5
		Ga2	1096	0.085	0.090	0.077	0.065	0.056	0.050	0.046	1118	1058	1110	1076	0	10
Germanium	Ge	Ge4	55	0.120	0.098	0.062	0.046	0.039	0.032	0.029	78	18	70	36	0	35
		Ge3	1047	0.045	0.055	0.049	0.041	0.037	0.032	0.029	1068.5	1008.5	1060.5	1026.5	0	35
		Ge1	1150	0.172	0.212	0.184	0.157	0.137	0.122	0.112	1171.5	1111.5	1163.5	1129.5	3	10
		Ge2	1181	0.078	0.098	0.085	0.073	0.064	0.057	0.052	1202	1142	1194	1160	0	20
Gold	Au	Au1	74	0.873	0.738	0.527	0.393	0.319	0.271	0.239	96	36	88	54	0	5
		Au2	243	0.064	0.059	0.044	0.035	0.028	0.025	0.023	264.5	204.5	256.5	222.5	0	40
		Au6	1522	0.005	0.010	0.011	0.011	0.010	0.008	0.008	1524	1464	1516	1482	0	175
		Au5	1771	0.010	0.018	0.022	0.019	0.018	0.017	0.016	1789	1729	1781	1747	0	90
		Au3	2022	0.026	0.054	0.064	0.058	0.053	0.048	0.045	2040	1980	2032	1998	3	25
		Au4	2107	0.013	0.037	0.047	0.043	0.038	0.035	0.033	2125	2065	2117	2083	0	35
Hafnium	Hf	Hf1	184	0.154	0.133	0.082	0.063	0.053	0.044	0.040	195	135	187	153	0	20
		Hf4	1231	0.008	0.013	0.013	0.011	0.010	0.009	0.008	1241	1181	1233	1199	0	115
		Hf3	1427	0.016	0.028	0.026	0.023	0.020	0.018	0.017	1433	1373	1425	1391	0	60
		Hf2	1625	0.055	0.087	0.080	0.071	0.063	0.057	0.052	1644	1584	1636	1602	3	20
Holmium	Ho	Ho1	162	0.210	0.164	0.096	0.072	0.061	0.052	0.046	175	115	167	133	0	30
		Ho3	1016	0.028	0.035	0.030	0.025	0.022	0.020	0.019	1020	960	1012	978	0	85
		Ho2	1177	0.048	0.059	0.050	0.043	0.037	0.034	0.031	1186	1126	1178	1144	3	50
		Ho4	1339	0.029	0.035	0.029	0.026	0.022	0.020	0.019	1354	1294	1346	1312	0	85
Indium	In	In1	405	1.113	0.912	0.671	0.532	0.448	0.390	0.347	428	368	420	386	3	5
Iodine	I	I1	510	0.453	0.432	0.485	0.392	0.332	0.292	0.262	531	471	523	489	3	5
		I2	519	0.452	0.407	0.431	0.348	0.297	0.260	0.234	541	481	533	499	0	5
		I3	562	0.053	0.062	0.062	0.050	0.042	0.036	0.033	584.5	524.5	576.5	542.5	0	35

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Iridium	Ir	Ir1	175	0.097	0.081	0.054	0.042	0.036	0.032	0.028	188	128	180	146	0	30
		Ir4	233	0.060	0.051	0.032	0.026	0.020	0.018	0.016	254	194	246	212	0	50
		Ir6	1439	0.005	0.011	0.011	0.010	0.010	0.008	0.007	1443	1383	1435	1401	0	145
		Ir5	1672	0.013	0.021	0.021	0.018	0.017	0.016	0.015	1690	1630	1682	1648	0	85
		Ir2	1909	0.032	0.064	0.066	0.060	0.054	0.050	0.046	1926	1866	1918	1884	3	25
		Ir3	1982	0.021	0.047	0.049	0.046	0.041	0.038	0.035	2000	1940	1992	1958	0	30
Iron	Fe	Fe4	50	0.751	0.577	0.355	0.263	0.213	0.180	0.157	73	13	65	31	0	5
		Fe1	600	0.112	0.108	0.081	0.066	0.056	0.049	0.045	616	556	608	574	3	15
		Fe2	654	0.164	0.158	0.116	0.094	0.081	0.072	0.064	672.5	612.5	664.5	630.5	0	10
		Fe3	705	0.195	0.190	0.137	0.112	0.096	0.084	0.075	727.5	667.5	719.5	685.5	0	10
Lanthanum	La	La1	83	1.008	0.701	0.433	0.334	0.275	0.236	0.209	105	45	97	63	0	10
		La2	634	0.140	0.130	0.102	0.085	0.073	0.064	0.059	644	584	636	602	3	25
		La3	732	0.047	0.043	0.033	0.027	0.024	0.020	0.018	736.5	676.5	728.5	694.5	0	70
Lead	Pb	Pb1	97	1.169	1.002	0.657	0.498	0.407	0.350	0.307	119	59	111	77	3	5
		Pb2	251	0.064	0.061	0.043	0.033	0.028	0.024	0.021	272	212	264	230	0	60
		Pb6	1641	—	0.006	0.009	0.007	0.007	0.006	0.006	1638	1578	1630	1596	0	340
		Pb5	1914	0.006	0.015	0.017	0.016	0.015	0.014	0.013	1910	1850	1902	1868	0	145
		Pb3	2188	0.008	0.032	0.037	0.034	0.032	0.029	0.027	2201	2141	2193	2159	0	60
		Pb4	2288	—	0.002	0.023	0.022	0.021	0.019	0.018	2303.5	2243.5	2295.5	2261.5	0	85
Lithium	Li	Li1	57	0.046	0.027	0.009	0.007	0.005	0.005	0.004	72	12	64	30	3	55
Lutetium	Lu	Lu1	182	0.232	0.186	0.112	0.086	0.071	0.060	0.053	194	134	186	152	0	25
		Lu4	1188	0.018	0.024	0.019	0.017	0.016	0.014	0.013	1198	1138	1190	1156	0	135
		Lu3	1378	0.030	0.042	0.036	0.031	0.027	0.025	0.023	1384	1324	1376	1342	0	75
		Lu2	1568	0.085	0.122	0.106	0.092	0.083	0.075	0.068	1586	1526	1578	1544	3	25
Magnesium	Mg	Mg1	48	0.953	0.711	0.439	0.323	0.261	0.221	0.192	71	11	63	29	0	10
		Mg2	1188	0.096	0.120	0.109	0.092	0.081	0.073	0.066	1199	1139	1191	1157	3	10
Manganese	Mn	Mn4	45	0.588	0.427	0.261	0.193	0.155	0.131	0.115	67	7	59	25	0	5
		Mn1	545	0.151	0.139	0.098	0.079	0.068	0.059	0.053	561	501	553	519	3	10
		Mn2	592	0.194	0.175	0.128	0.103	0.088	0.077	0.069	611	551	603	569	0	10
		Mn3	638	0.148	0.133	0.097	0.078	0.066	0.059	0.052	660	600	652	618	0	10

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Mercury	Hg	Hg1	81	1.112	0.916	0.614	0.462	0.376	0.320	0.281	103	43	95	61	3	5
		Hg2	246	0.068	0.059	0.043	0.033	0.028	0.024	0.021	268	208	260	226	0	60
		Hg5	1818	0.011	0.020	0.021	0.020	0.018	0.017	0.015	1836	1776	1828	1794	0	110
		Hg3	2078	0.029	0.044	0.051	0.047	0.042	0.039	0.036	2093	2033	2085	2051	0	40
		Hg4	2166	0.020	0.028	0.036	0.033	0.031	0.028	0.026	2184	2124	2176	2142	0	55
Molybdenum	Mo	Mo1	190	0.389	0.308	0.192	0.148	0.122	0.105	0.093	212	152	204	170	3	10
		Mo3	225	0.333	0.266	0.164	0.127	0.104	0.090	0.079	247	187	239	205	0	10
		Mo5	1881	0.004	0.008	0.009	0.008	0.008	0.007	0.007	1899	1839	1891	1857	0	145
		Mo2	2044	0.008	0.026	0.029	0.027	0.025	0.023	0.022	2062	2002	2054	2020	0	45
		Mo4	2149	0.003	0.011	0.013	0.012	0.011	0.010	0.010	2167	2107	2159	2125	0	90
Neodymium	Nd	Nd1	96	0.857	0.617	0.398	0.299	0.245	0.209	0.184	118	58	110	76	0	10
		Nd2	734	0.101	0.099	0.083	0.069	0.060	0.053	0.048	751	691	743	709	3	30
		Nd3	861	0.039	0.039	0.031	0.026	0.023	0.020	0.018	863	803	855	821	0	75
Nickel	Ni	Ni4	64	0.485	0.380	0.247	0.182	0.147	0.126	0.110	84	24	76	42	0	5
		Ni3	718	0.047	0.050	0.040	0.033	0.028	0.025	0.023	733	673	725	691	0	25
		Ni2	785	0.076	0.080	0.065	0.053	0.046	0.041	0.037	799	739	791	757	0	15
		Ni1	849	0.202	0.210	0.170	0.141	0.121	0.107	0.097	871	811	863	829	3	5
Niobium	Nb	Nb1	170	0.443	0.358	0.235	0.180	0.149	0.129	0.113	192.5	132.5	184.5	150.5	3	5
		Nb3	201	0.230	0.184	0.121	0.093	0.076	0.066	0.058	223.5	163.5	215.5	181.5	0	15
		Nb5	1787	0.005	0.011	0.012	0.011	0.010	0.010	0.008	1787	1727	1779	1745	0	125
		Nb2	1944	0.011	0.026	0.032	0.030	0.027	0.025	0.023	1962	1902	1954	1920	0	45
		Nb4	2039	0.007	0.012	0.014	0.014	0.013	0.012	0.011	2056	1996	2048	2014	0	90
Nitrogen	N	N1	389	0.227	0.171	0.113	0.089	0.074	0.064	0.057	407	347	399	365	3	10
Osmium	Os	Os1	180	0.114	0.079	0.051	0.040	0.033	0.029	0.026	191	131	183	149	0	30
		Os4	226	0.049	0.034	0.022	0.016	0.014	0.012	0.011	247	187	239	205	0	65
		Os6	1396	0.007	0.010	0.010	0.008	0.007	0.007	0.006	1402	1342	1394	1360	0	160
		Os5	1622	0.012	0.017	0.017	0.015	0.013	0.012	0.011	1640	1580	1632	1598	0	95
		Os2	1850	0.044	0.063	0.064	0.058	0.052	0.047	0.044	1869	1809	1861	1827	3	25
		Os3	1920	0.028	0.041	0.043	0.039	0.036	0.032	0.030	1938	1878	1930	1896	0	35
Oxygen	O	O1	510	0.171	0.152	0.109	0.088	0.073	0.064	0.057	532	472	524	490	3	5

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Palladium	Pd	Pd2	283	0.180	0.157	0.112	0.088	0.072	0.063	0.057	300	240	292	258	0	15
		Pd1	333	1.017	0.886	0.630	0.493	0.411	0.356	0.316	352.5	292.5	344.5	310.5	3	5
		Pd5	2282	–	0.004	0.004	0.004	0.004	0.004	0.004	2300	2240	2292	2258	0	270
Phosphorus	P	P1	123	1.259	0.934	0.567	0.427	0.350	0.298	0.262	145.5	85.5	137.5	103.5	3	5
		P2	1862	0.027	0.052	0.055	0.051	0.046	0.042	0.039	1880	1820	1872	1838	0	25
Platinum	Pt	Pt1	70	0.624	0.477	0.360	0.268	0.216	0.183	0.161	89	29	81	47	3	5
		Pt2	173	0.055	0.045	0.036	0.028	0.023	0.020	0.017	195	135	187	153	0	50
		Pt3	241	0.052	0.042	0.032	0.025	0.021	0.017	0.016	261.5	201.5	253.5	219.5	0	50
		Pt7	1484	0.004	0.010	0.011	0.010	0.008	0.008	0.007	1487	1427	1479	1445	0	175
		Pt6	1725	0.011	0.016	0.021	0.018	0.017	0.016	0.015	1743	1683	1735	1701	0	90
		Pt4	1969	0.028	0.053	0.063	0.059	0.053	0.048	0.045	1987	1927	1979	1945	3	25
		Pt5	2048	0.019	0.042	0.051	0.047	0.043	0.040	0.037	2067	2007	2059	2025	0	30
Potassium	K	K1	252	1.160	0.990	0.747	0.580	0.482	0.417	0.369	272	212	264	230	3	5
Praseodymium	Pr	Pr1	91	0.872	0.643	0.399	0.299	0.244	0.209	0.183	113.5	53.5	105.5	71.5	0	10
		Pr2	696	0.085	0.085	0.066	0.055	0.047	0.042	0.038	714	654	706	672	3	35
		Pr3	817	0.037	0.034	0.026	0.022	0.018	0.016	0.015	820	760	812	778	0	85
Rhenium	Re	Re1	179	0.166	0.134	0.085	0.066	0.055	0.048	0.042	188	128	180	146	0	15
		Re4	218	0.061	0.048	0.030	0.023	0.019	0.017	0.015	240	180	232	198	0	45
		Re6	1354	0.008	0.013	0.012	0.011	0.009	0.009	0.008	1361	1301	1353	1319	0	120
		Re5	1572	0.013	0.022	0.022	0.019	0.017	0.016	0.015	1590	1530	1582	1548	0	70
		Re2	1793	0.047	0.080	0.078	0.071	0.064	0.058	0.053	1812	1752	1804	1770	3	20
		Re3	1858	0.028	0.049	0.048	0.044	0.039	0.035	0.033	1877	1817	1869	1835	0	30
Rhodium	Rh	Rh2	259	0.246	0.212	0.155	0.121	0.100	0.087	0.078	278	218	270	236	0	10
		Rh1	305	0.916	0.783	0.572	0.446	0.370	0.321	0.285	326	266	318	284	3	5
		Rh5	2180	–	0.004	0.005	0.005	0.005	0.005	0.004	2197	2137	2189	2155	0	230
		Rh3	2366	–	0.008	0.014	0.014	0.013	0.012	0.012	2381	2321	2373	2339	0	70

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Rubidium	Rb	Rb5	78	0.335	0.254	0.184	0.138	0.112	0.095	0.085	98.5	38.5	90.5	56.5	0	45
		Rb4	107	0.142	0.102	0.074	0.056	0.047	0.040	0.035	128.5	68.5	120.5	86.5	0	105
		Rb3	1433	0.011	0.018	0.022	0.019	0.017	0.016	0.014	1438	1378	1430	1396	0	210
		Rb1	1561	0.044	0.062	0.080	0.072	0.064	0.058	0.053	1579	1519	1571	1537	3	60
		Rb2	1620	0.022	0.029	0.040	0.037	0.033	0.029	0.027	1639	1579	1631	1597	0	125
Ruthenium	Ru	Ru2	235	0.236	0.204	0.124	0.097	0.081	0.069	0.062	255	195	247	213	0	10
		Ru1	277	0.612	0.527	0.322	0.250	0.207	0.179	0.159	299	239	291	257	3	5
		Ru5	2078	—	0.005	0.005	0.005	0.005	0.004	0.004	2063	2003	2055	2021	0	210
		Ru3	2256	—	0.016	0.018	0.017	0.017	0.016	0.015	2273	2213	2265	2231	0	60
		Ru4	2385	—	0.006	0.008	0.007	0.007	0.006	0.006	2401	2341	2393	2359	0	120
Samarium	Sm	Sm1	103	0.496	0.370	0.240	0.182	0.148	0.127	0.112	125.5	65.5	117.5	83.5	0	15
		Sm3	135	0.246	0.176	0.106	0.082	0.068	0.059	0.052	145.5	85.5	137.5	103.5	0	30
		Sm2	814	0.065	0.068	0.055	0.046	0.040	0.036	0.032	826	766	818	784	3	45
		Sm4	940	0.047	0.050	0.039	0.034	0.029	0.026	0.024	952	892	944	910	0	60
Scandium	Sc	Sc1	343	0.378	0.311	0.210	0.166	0.139	0.120	0.107	362	302	354	320	3	10
		Sc2	370	0.390	0.321	0.215	0.170	0.142	0.123	0.110	393	333	385	351	0	10
Selenium	Se	Se5	47	0.056	0.045	0.051	0.036	0.031	0.025	0.022	69	9	61	27	2	55
		Se4	104	0.058	0.045	0.019	0.015	0.011	0.010	0.010	122	62	114	80	0	140
		Se3	1192	0.027	0.036	0.010	0.009	0.008	0.007	0.007	1213	1153	1205	1171	0	160
		Se1	1311	0.102	0.133	0.044	0.039	0.034	0.030	0.028	1331	1271	1323	1289	3	40
		Se2	1352	0.053	0.063	0.022	0.019	0.017	0.015	0.014	1372	1312	1364	1330	0	85
Silicon	Si	Si1	96	0.698	0.681	0.423	0.316	0.257	0.219	0.193	118	58	110	76	0	5
		Si3	96	0.117	0.104	0.087	0.066	0.053	0.044	0.039	118	58	110	76	0	5
		Si2	1621	0.035	0.073	0.077	0.068	0.061	0.055	0.050	1640	1580	1632	1598	3	20
		Si4	1621	0.034	0.056	0.068	0.060	0.054	0.049	0.045	1640	1580	1632	1598	0	20

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Silver	Ag	Ag1	359	1.212	1.063	0.767	0.603	0.504	0.438	0.389	376.5	316.5	368.5	334.5	3	5
		Ag4	2381	–	0.002	0.004	0.004	0.004	0.004	0.003	2399	2339	2391	2357	0	285
Sodium	Na	Na1	996	0.089	0.097	0.086	0.071	0.061	0.055	0.049	1011	951	1003	969	3	20
Strontium	Sr	Sr4	114	0.198	0.139	0.100	0.078	0.065	0.056	0.049	135	75	127	93	0	45
		Sr3	1516	0.012	0.015	0.017	0.016	0.015	0.012	0.012	1520	1460	1512	1478	0	190
		Sr1	1651	0.039	0.057	0.067	0.060	0.054	0.049	0.045	1665	1605	1657	1623	3	50
		Sr2	1718	0.017	0.022	0.027	0.024	0.022	0.021	0.018	1731	1671	1723	1689	0	125
Sulfur	S	S1	153	2.179	1.777	1.113	0.847	0.695	0.596	0.526	174.5	114.5	166.5	132.5	3	5
		S2	2119	0.015	0.028	0.036	0.034	0.031	0.029	0.027	2136	2076	2128	2094	0	45
Tantalum	Ta	Ta1	183	0.188	0.155	0.106	0.082	0.068	0.059	0.052	193	133	185	151	0	15
		Ta4	1271	0.008	0.013	0.014	0.012	0.010	0.009	0.009	1280	1220	1272	1238	0	100
		Ta3	1475	0.016	0.027	0.028	0.025	0.023	0.020	0.019	1479	1419	1471	1437	0	50
		Ta2	1680	0.051	0.083	0.088	0.078	0.069	0.063	0.058	1699	1639	1691	1657	3	15
Tellurium	Te	Te1	486	0.722	0.659	0.507	0.409	0.347	0.304	0.272	507	447	499	465	3	5
Terbium	Tb	Tb1	116	0.267	0.148	0.089	0.067	0.056	0.048	0.041	139	79	131	97	0	35
		Tb3	150	0.319	0.172	0.098	0.074	0.060	0.051	0.045	167	107	159	125	0	30
		Tb4	937	0.049	0.041	0.033	0.027	0.024	0.022	0.020	943	883	935	901	0	75
		Tb2	1078	0.056	0.050	0.039	0.033	0.029	0.026	0.023	1091	1031	1083	1049	3	65
		Tb5	1230	0.023	0.017	0.014	0.011	0.010	0.009	0.008	1247	1187	1239	1205	0	190
Thallium	Tl	Tl1	90	1.175	1.066	0.665	0.502	0.409	0.351	0.308	111.5	51.5	103.5	69.5	3	5
		Tl2	250	0.058	0.057	0.036	0.029	0.024	0.021	0.019	270	210	262	228	0	70
		Tl6	1601	–	0.007	0.007	0.007	0.006	0.006	0.006	1600	1540	1592	1558	0	330
		Tl5	1865	0.009	0.016	0.016	0.015	0.014	0.013	0.012	1863	1803	1855	1821	0	145
		Tl3	2132	0.014	0.039	0.040	0.038	0.034	0.032	0.030	2147	2087	2139	2105	0	55
		Tl4	2227	0.009	0.024	0.026	0.025	0.023	0.021	0.020	2243	2183	2235	2201	0	75

\* Peak labeling (e.g., 0 = “none”.)

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### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Thorium	Th	Th1	69	0.875	0.705	0.463	0.362	0.303	0.263	0.234	91.5	31.5	83.5	49.5	3	5
		Th2	249	0.092	0.088	0.065	0.053	0.045	0.040	0.036	271.5	211.5	263.5	229.5	0	25
		Th5	2296	–	0.002	0.003	0.003	0.003	0.003	0.003	2311	2251	2303	2269	0	420
Thulium	Tm	Tm1	170	0.243	0.173	0.116	0.088	0.073	0.063	0.056	179	119	171	137	3	25
		Tm4	1100	0.028	0.031	0.029	0.026	0.022	0.020	0.018	1108	1048	1100	1066	0	85
		Tm3	1278	0.042	0.045	0.045	0.039	0.035	0.031	0.029	1285	1225	1277	1243	0	55
		Tm2	1452	0.065	0.078	0.074	0.065	0.056	0.052	0.047	1469	1409	1461	1427	3	35
Tin	Sn	Sn1	432	1.094	1.020	0.737	0.587	0.496	0.433	0.387	454	394	446	412	3	5
Titanium	Ti	Ti1	390	0.327	0.276	0.190	0.151	0.126	0.111	0.099	408	348	400	366	0	5
		Ti2	421	0.510	0.432	0.293	0.232	0.195	0.170	0.152	444	384	436	402	3	5
Tungsten	W	W1	182	0.186	0.150	0.096	0.075	0.062	0.053	0.047	193	133	185	151	0	15
		W5	210	0.038	0.029	0.019	0.015	0.013	0.011	0.010	232	172	224	190	0	70
		W4	1312	0.011	0.015	0.015	0.013	0.012	0.011	0.011	1320	1260	1312	1278	0	100
		W3	1524	0.019	0.027	0.025	0.023	0.021	0.018	0.017	1527	1467	1519	1485	0	60
		W2	1737	0.056	0.088	0.088	0.079	0.071	0.064	0.059	1755	1695	1747	1713	3	15
Uranium	U	U1	77	1.035	0.761	0.524	0.413	0.345	0.300	0.268	99.5	39.5	91.5	57.5	3	5
		U2	284	0.217	0.188	0.149	0.122	0.105	0.093	0.084	307	247	299	265	0	10
Vanadium	V	V1	440	0.244	0.215	0.154	0.123	0.104	0.090	0.081	457	397	449	415	0	10
		V2	475	0.380	0.332	0.234	0.187	0.157	0.138	0.123	497	437	489	455	3	5
Ytterbium	Yb	Yb1	174	0.256	0.185	0.141	0.108	0.089	0.076	0.067	187	127	179	145	0	25
		Yb4	1141	0.021	0.027	0.029	0.025	0.023	0.020	0.018	1155	1095	1147	1113	0	115
		Yb3	1329	0.033	0.040	0.045	0.040	0.035	0.032	0.029	1334	1274	1326	1292	0	75
		Yb2	1511	0.086	0.109	0.119	0.104	0.092	0.084	0.076	1526	1466	1518	1484	3	30
Yttrium	Y	Y1	132	0.342	0.277	0.164	0.127	0.105	0.091	0.082	155.5	95.5	147.5	113.5	0	20
		Y4	1606	0.007	0.015	0.015	0.013	0.012	0.011	0.010	1608	1548	1600	1566	0	160
		Y2	1748	0.024	0.051	0.051	0.046	0.042	0.039	0.035	1764	1704	1756	1722	3	45
		Y3	1823	0.012	0.023	0.023	0.020	0.019	0.017	0.015	1840	1780	1832	1798	0	105

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

### C: AES Sensitivity Factors

Element	Region	Peak	Sensitivity Factor ( $S_x$ )							Acquisition		Analysis		*	†	
			3 keV	5 keV	10 keV	15 keV	20 keV	25 keV	30 keV	High	Low	High	Low			
Zinc	Zn	Zn4	64	0.424	0.338	0.236	0.177	0.144	0.123	0.107	86	26	78	44	0	5
		Zn3	839	0.034	0.038	0.036	0.029	0.026	0.023	0.020	853	793	845	811	0	35
		Zn2	908	0.073	0.081	0.077	0.065	0.056	0.050	0.046	930.5	870.5	922.5	888.5	0	15
		Zn1	997	0.241	0.279	0.262	0.219	0.190	0.169	0.154	1018	958	1010	976	3	5
Zirconium	Zr	Zr1	151	0.609	0.491	0.337	0.263	0.219	0.191	0.170	173.5	113.5	165.5	131.5	3	5
		Zr4	1695	0.010	0.017	0.022	0.019	0.018	0.017	0.016	1697	1637	1689	1655	0	90
		Zr2	1844	0.025	0.051	0.060	0.056	0.051	0.046	0.043	1861	1801	1853	1819	0	30
		Zr3	1929	0.008	0.022	0.028	0.025	0.023	0.021	0.020	1946	1886	1938	1904	0	65

\* Peak labeling (e.g., 0 = "none".)

† Number of sweeps.

# Appendix D: Conversion of Apollo Data Files

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This appendix describes (1) how to translate PHI data files created on an Apollo computer into a MultiPak-readable format, and (2) how to transfer the translated files to a PC.

## Translating Apollo Files

Install PHIC (shipped with MultiPak) on your Apollo computer. Instructions for installation accompany the PHIC package.

At the prompt on the Apollo, type:

**phic  $\wedge$  -tpak  $\wedge$  <filename>**      ( $\wedge$  = space;  
 $<\text{filename}>$  = complete Apollo  
name of the file)

The PHIC routine creates a new file or set of files named for the original Apollo file and with a three-character MultiPak extension added (e.g., spe, pro, ang, etc.) PHIC creates a file for each analysis point (point or area or line) in the original data file. In this case, an underscore (“\_”) and numeral (e.g., 1, 2, etc.) are added after the file name and before the extension.

For example, a survey spectrum (taken on a PHI system using an Apollo computer) that had three analysis points and four regions generated one Apollo file, named datacu12.mat. When translated by PHIC, it created one data file for each of the analysis points. Each new data file contains data from four regions at that analysis point.

Apollo File Name	New File Names
datacu12.mat	datacu_1.spe; datacu_2.spe; datacu_3.spe

## Transferring Translated Files

The Apollo computer and the PC on which MultiPak resides need to be networked together to transfer the files. The following procedure is intended to guide the operator through the process.

1. On the Apollo computer, configure the Ethernet interface for using the AUI port (15-pin connector at the rear) as follows:
  - If you have a 425e Apollo, open the top cover and move the jumper block located toward the rear of the CPU to the set pins located closest to the front panel.
  - If you have a DN type computer, set the blue or black jumper block to the DIS position.
2. Next, install the 10-BASE-T transceiver onto the AUI connector. Run cross-over twisted-pair cable\* from the transceiver to the Ethernet connector on the PC.
3. On the Apollo, enter the following at the login and password prompts:

*Login*            **root**

*Password*        **-apollo-**

4. At the next two prompts, type the following to create TCP/IP daemon stub files:

**cd /etc/daemons**

**touch \_tcpd \_inetd**

5. Edit “/etc/rc.local” to enable IP address broadcasting through TCP/IP as follows. Find the lines shown below in plain type, then add the lines shown below in bold after it:

```
# ifconfig eth0
ifconfig eth0
...
<ip-address>
128.1.1.203        netmask 255.255.255.0
```

---

\* This cable can be ordered from Physical Electronics. Specify part number 628223.

6. Create and edit “/etc/hosts” by typing the following:

```
#Loopback
#
127.0.0.1      localhost
255.255.255.0  subnetmask
#
#
#
#Ethernet subnet
128.1.1.200    phi1
128.1.1.201    phi2
128.1.1.203    nxxxxxx      (xxxxxx = node id of the Apollo)
128.1.1.200    nt-node     (nt-node = PC name as listed on
                                Program Manager title bar—without
                                spaces.)
```

7. Set up TCP/IP support on the PC using Windows NT as follows:
  - Login as **Administrator** (no password).
  - In Program Manager, open Main Group—Control Panel—Network.
  - Click on “Add Software.” Click on the scroll bar and select “TCP/IP Protocol and Related Components.” Press Continue.
  - Select “Simple TCP/IP Services.” Insert the Windows NT CD-ROM. Change the directory to d:/i386. Press OK.
  - In “TCP/IP Configuration,” do the following:
    - Move the cursor to the left-most dot.
    - Insert **128.1.1.210**.
    - Press the Tab key.
    - Subnet Mask = **255.255.0.0**.
    - Press OK.
8. Reboot both computers.
9. Edit the “hosts” file on the PC as follows:
  - Open Notepad.
  - Open the file. Its path is c:\winnt35\system32\drivers\etc\hosts.
  - Add the following line at the end of the file:

**128.1.1.203 nxxxxxx** (*xxxxxx = node id of the Apollo*)

## **D: Conversion of Apollo Data Files**

- d. Save the file.

10. Using the PC, transfer the files from the Apollo to the PC as follows:

- a. Click on the MS-DOS Prompt icon to open it.

b. At the DOS prompt, type:

```
cd \usr\userdata\data\<yourdata>
```

**ftp nxxxxxx** (*xxxxxx = node id of Apollo*)

c. When the DOS prompt changes to “ftp> login:” type the following:

user

d. Press Enter when prompted for a password.

e. At the following “ftp>“ prompts, type the following lines:

```
cd /usr/datafile
```

**binary** *(The transfer must be binary.)*

## **prompt**

**mget** filename OR **mput** \* (\* = *all files*)

quit

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