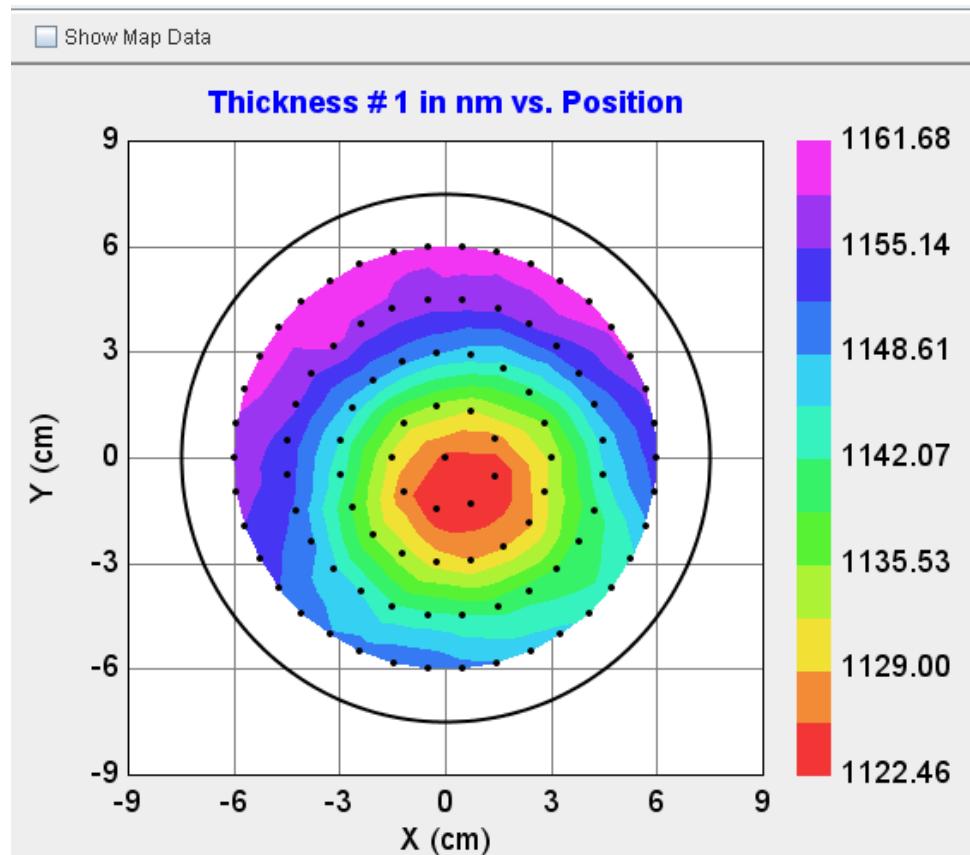


---

Version 4.05

# CompleteEASE™ Data Analysis Manual

By J. A. Woollam Co., Inc.  
June 25, 2009



**Copyright © 2004-2009 J. A. Woollam Co., Inc. All Rights Reserved.**

## **J. A. Woollam Co., Inc.**

645 M Street, Suite 102  
Lincoln, NE 68508

Internet:      sales@jawoollam.com  
                  support@jawoollam.com  
Website:        <http://www.jawoollam.com>  
Phone:           402.477.7501  
Fax:             402.477.8214

### **Trademarks**

CompleteEASE™ is a trademark of the J. A. Woollam Co., Inc. All other trademarks used within are the property of their respective owners.

### **Copying and Distribution**

You are welcome to make backup copies of the CompleteEASE software and documentation for your own use and protection. However, you are not permitted to make copies for others or for resale.

# Contents

|           |  |           |
|-----------|--|-----------|
| <b>1.</b> | <b>Introduction</b>                        | <b>1</b>  |
| 1.1.      | New Features of Interest.....              | 1         |
|           | Snapshots.....                             | 1         |
|           | 3-Deep File Structure .....                | 1         |
|           | Multi-Processor Capability.....            | 2         |
|           | Model “roll-back”.....                     | 2         |
|           | Anisotropic Modeling.....                  | 3         |
|           | New Mapping Features.....                  | 3         |
|           | Easy access to manual .....                | 4         |
| 1.2.      | Manual Overview .....                      | 5         |
| 1.3.      | Installing the Software.....               | 7         |
|           | Before Installation .....                  | 7         |
|           | Running the SETUP Program .....            | 7         |
| 1.4.      | Conventions Used in this Manual.....       | 10        |
|           | Tabs .....                                 | 10        |
|           | Screen Panels.....                         | 10        |
|           | Buttons .....                              | 10        |
|           | Model Commands .....                       | 11        |
|           | Mouse-selected Menus .....                 | 11        |
|           | Pipelining Descriptions .....              | 12        |
| 1.5.      | File Structure .....                       | 13        |
|           | COMMON Location .....                      | 14        |
|           | Folder “Links” .....                       | 14        |
| 1.6.      | Setting Up Multiple Users .....            | 19        |
| 1.7.      | Short-cut Guide .....                      | 21        |
| 1.8.      | What is Spectroscopic Ellipsometry? .....  | 22        |
| <b>2.</b> | <b>Data Collection</b>                     | <b>24</b> |
| 2.1.      | alpha-SE Systems .....                     | 24        |
|           | Common Models .....                        | 25        |
|           | Measuring a Sample .....                   | 26        |
| 2.2.      | M-2000, RC2, and AccuMap-SE Systems .....  | 29        |
|           | Measurement Recipe .....                   | 29        |
| 2.3.      | Acquisition Parameters.....                | 33        |
|           | Data Type .....                            | 33        |
|           | Sample Alignment.....                      | 34        |
|           | Common Acquisition Parameters.....         | 37        |
| 2.4.      | Scan Pattern.....                          | 38        |
|           | Adding COMMON Scan Patterns .....          | 39        |
| 2.5.      | Model .....                                | 40        |
|           | Common Models .....                        | 40        |
| 2.6.      | Running a Recipe and Viewing Results ..... | 41        |

|   |           |
|---|-----------|
| <b>3. Data Analysis 1 – Basic</b>                         | <b>44</b> |
| 3.1. General Data Analysis Theory .....                   | 46        |
| “Pseudo” Optical Constants.....                           | 47        |
| Layered Optical Model.....                                | 47        |
| “Goodness” of Fit: definition of the MSE .....            | 49        |
| “Fitting” the Data .....                                  | 50        |
| Evaluating the Fit Results.....                           | 51        |
| “Physical” Optical Constants.....                         | 52        |
| 3.2. Samples with Known N,K: SiO <sub>2</sub> on Si ..... | 54        |
| Fit Results and Parameter Error Bars .....                | 55        |
| JAW Oxide on Si Model, with Interfacial Layer.....        | 57        |
| Derived Parameters .....                                  | 57        |
| Hiding, Renaming, and Bounding Fit Parameters .....       | 58        |
| Thickness Pre-fitting .....                               | 59        |
| Visualizing Model Changes .....                           | 62        |
| 3.3. Transparent Thin Films - 1 .....                     | 63        |
| Si with Transparent Film .....                            | 64        |
| Global Fits .....   | 66        |
| 3.4. Transparent Substrates.....                          | 68        |
| Backside Substrate Reflections .....                      | 68        |
| Graphing Multiple Data Sets .....                         | 69        |
| Using the Graph ScratchPad.....                           | 70        |
| Graphing Depolarization .....                             | 73        |
| Including Backside reflections .....                      | 75        |
| Fitting Depolarization.....                               | 75        |
| 3.5. Transparent Films - 2.....                           | 79        |
| Glass with Transparent Film.....                          | 79        |
| Surface Roughness .....                                   | 81        |
| Graded Index .....  | 81        |
| <u>Try Alternate Models</u> .....                         | 83        |
| 3.6. Log and Report a Series of Films .....               | 85        |
| Copy to Clipboard .....                                   | 86        |
| HTML Clipboard.....                                       | 87        |
| Fit Log .....   | 87        |
| Comparing Results .....                                   | 88        |
| Compare Optical Constants.....                            | 89        |
| Re-analyzing Multiple Data Sets .....                     | 90        |
| ‘Generate Report’ .....                                   | 90        |
| Save Log File.....  | 92        |
| Snapshot .....  | 92        |
| <b>4. Data Analysis 2 - Intermediate</b>                  | <b>93</b> |
| 4.1. Metal Substrates .....                               | 95        |
| <u>Save</u> .....   | 98        |
| Save Layer Optical Constants.....                         | 98        |
| Au Substrate Model.....                                   | 99        |
| 4.2. Self Assembled Monolayer on Au .....                 | 100       |
| Self-Assembled Monolayers.....                            | 100       |
| <u>Parameter Uniqueness</u> .....                         | 101       |
| 4.3. Absorbing Thin Films (B-SPLINE) .....                | 104       |
| Identifying an Absorbing Film .....                       | 104       |
| Si with Absorbing Film .....                              | 105       |
| The “B-Spline” Layer.....                                 | 107       |
| Wavelength Range Expansion (WVL-EXPAND) Fit .....         | 109       |

|           |  |            |
|-----------|--|------------|
|           | WVL-EXPAND Fit with B-SPLINE Layer .....                                     | 111        |
|           | Global Fits with WVL-EXPAND Fitting .....                                    | 111        |
| 4.4.      | Absorbing Thin Films (Gen-Osc).....  | 113        |
|           | Parameterize Layer .....   | 113        |
|           | Glass with Absorbing Film.....   | 122        |
| 4.5.      | Multiple Layer Film Stacks .....   | 128        |
|           | Oxide or Roughness?.....   | 131        |
| 4.6.      | Multiple Data Types (SE + T).....  | 132        |
|           | <u>Parameter Uniqueness</u> .....  | 132        |
|           | Append Data.....   | 133        |
|           | Transmission Data % Weight.....  | 134        |
| <b>5.</b> | <b>Data Analysis 3 – Advanced</b>  | <b>137</b> |
| 5.1.      | Map Data and Model Non-Idealities .....                                      | 139        |
|           | Show Map Data .....  | 139        |
|           | Selecting a Point from the Map .....   | 140        |
|           | Silicon with Transparent Film .....  | 140        |
|           | Wavelength Units – eV .....  | 140        |
|           | Fixing Cauchy Dispersion .....   | 142        |
|           | ‘Set Ranges’ .....   | 142        |
|           | Sellmeier.....   | 143        |
|           | Fit Scan Data .....  | 144        |
|           | Model Calculation .....  | 145        |
|           | Model Calculation – Thickness Non-Uniformity .....                           | 146        |
|           | Model Calculation – Bandwidth (nm) .....                                     | 147        |
|           | Include Depolarization Data.....   | 148        |
| 5.2.      | Multi-Sample Analysis .....  | 150        |
|           | Short-Cuts for Mapping Data .....  | 151        |
|           | Multi-Layer (empty) Model .....  | 151        |
|           | Set Symbol Size.....   | 152        |
|           | Zooming on Map .....   | 153        |
|           | Selecting Multiple Points on a Map .....                                     | 154        |
|           | Changing the Graph.....  | 155        |
|           | Graph All Data Sets.....   | 155        |
|           | Selecting and Unselecting Data Sets .....                                    | 156        |
|           | Multi-sample Analysis.....   | 157        |
|           | Clear Multi-Data Set Mode .....  | 158        |
|           | Multi-Sample Analysis (revisited).....                                       | 162        |
| 5.3.      | In Situ Data Analysis.....   | 168        |
|           | Short-Cuts for Dynamic Data .....  | 168        |
|           | Navigating In Situ Data .....  | 169        |
|           | Viewing Spectroscopic Data at a Specific Time .....                          | 169        |
|           | Turning off the “Auto-Fit” function .....                                    | 170        |
|           | Building a Model.....  | 171        |
|           | ‘Fit Dynamic’ .....  | 172        |
|           | Selecting Multiple Time-Slices .....   | 175        |
|           | Manipulating Multi-Data Sets .....   | 176        |
|           | Multi-Time Slice Analysis .....  | 177        |
|           | Fitting Optical Constants .....  | 179        |
| 5.4.      | Creating OC Library for Composition or Temperature-dependent materials ..... | 181        |
|           | Opt. Const. Compare Model.....   | 182        |
|           | <u>Draw Graph</u> .....  | 184        |
|           | <u>Save OC Library</u> .....   | 186        |
| 5.5.      | Anisotropic Films .....  | 188        |
|           | Convert to Anisotropic .....   | 190        |

|           |   |            |
|-----------|---|------------|
| 5.6.      | Biaxial Layer .....   | 190        |
| 5.6.      | Generalized SE and Mueller-Matrix Analysis.....               | 192        |
| <b>6.</b> | <b>Reference - Graph</b>                                      | <b>193</b> |
| 6.1.      | Basic Screen Layout .....                                     | 193        |
| 6.2.      | Graph Pane .....  | 194        |
|           | ‘Show Data’ .....   | 194        |
|           | Range-Select.....   | 194        |
|           | Zoom All .....  | 194        |
|           | Right-Click Menu (Graph) .....                                | 195        |
| <b>7.</b> | <b>Reference - Measurement Tab</b>                            | <b>198</b> |
| 7.1.      | System Status Panel.....                                      | 198        |
| 7.2.      | Measurement Controls Panel.....                               | 198        |
|           | Mode: .....   | 198        |
|           | Sample Alignment:.....  | 199        |
|           | Model .....   | 199        |
|           | Save Data after Measurement.....                              | 199        |
|           | ‘Measure’ .....   | 200        |
| 7.3.      | Fit Results Panel.....  | 200        |
| 7.4.      | Right-click menu ( <i>Measurement&gt;Fit Results:</i> ) ..... | 200        |
|           | Copy to Clipboard – Formatted .....                           | 200        |
|           | Copy to Clipboard - Table .....                               | 200        |
| 7.5.      | ‘View Previous Fit Results’ .....                             | 201        |
| <b>8.</b> | <b>Reference - Analysis Tab</b>                               | <b>203</b> |
| 8.1.      | Data: Panel .....   | 203        |
|           | ‘Open’ .....  | 203        |
|           | ‘Save’ .....  | 204        |
|           | ‘Info’ .....  | 204        |
|           | ‘Set Ranges’ .....  | 204        |
| 8.2.      | Fit: Panel .....  | 204        |
|           | ‘Generate’ .....  | 204        |
|           | ‘Fit’ .....   | 204        |
|           | ‘Fit Dynamic’ .....   | 205        |
|           | ‘Reset’ .....   | 205        |
| 8.3.      | Model: Panel.....   | 206        |
|           | ‘Open’ .....  | 206        |
|           | ‘Save’ .....  | 206        |
|           | ‘Clear’ .....   | 207        |
|           | <u>Add</u> .....  | 207        |
|           | <u>Delete</u> .....   | 207        |
|           | <u>Save</u> .....   | 208        |
|           | Include Surface Roughness .....                               | 208        |
|           | Model Pictorial .....   | 208        |
|           | Editing Layers .....  | 208        |
|           | Angle Offset .....  | 211        |
| 8.4.      | Right-click menu ( <i>Analysis&gt;Model:</i> ) .....          | 212        |
|           | Copy Model To Clipboard.....                                  | 212        |
|           | Copy Model To HTLM Clipboard .....                            | 213        |
|           | Copy Model (Layers Only) To Clipboard .....                   | 213        |
| 8.5.      | Layer types .....   | 214        |
|           | Tabulated n,k .....   | 215        |
|           | Void .....  | 215        |

|      |  |     |
|------|--|-----|
|      | EMA .....                                  | 215 |
|      | EMA-Coupled .....                          | 216 |
|      | Cauchy.....                                | 216 |
|      | Cauchy_WVL.....                            | 217 |
|      | Cauchy_Extended.....                       | 218 |
|      | The Sellmeier Layer .....                  | 218 |
|      | Coupled .....                              | 219 |
|      | WvlByWvl.....                              | 219 |
|      | Biaxial .....                              | 219 |
|      | Graded Layer.....                          | 220 |
|      | Gen-Osc.....                               | 221 |
|      | B-SPLINE .....                             | 223 |
|      | Intermix .....                             | 228 |
|      | Composition Library .....                  | 228 |
|      | Coupled .....                              | 229 |
|      | Uniaxial and Uniaxial-Diff.....            | 229 |
| 8.6. | Gen-Osc Oscillator Details.....            | 230 |
|      | e1 Offset .....                            | 230 |
|      | Pole .....                                 | 230 |
|      | Lorentz .....                              | 230 |
|      | Harmonic .....                             | 230 |
|      | Gaussian .....                             | 230 |
|      | Drude .....                                | 231 |
|      | Tauc-Lorentz and Cody-Lorentz .....        | 231 |
| 8.7. | +MODEL Options .....                       | 232 |
|      | Include Substrate Backside Correction..... | 232 |
|      | Model Calculation .....                    | 232 |
| 8.8. | +FIT Options .....                         | 234 |
|      | Perform Thickness Pre-Fit.....             | 235 |
|      | Use Global Fit .....                       | 235 |
|      | Selected Data.....                         | 235 |
|      | Fit Weight.....                            | 236 |
|      | Include Depolarization Data.....           | 236 |
|      | Include Intensity Data.....                | 236 |
|      | Transmission Data % Weight.....            | 236 |
|      | Limit Wvl. for Fit .....                   | 236 |
|      | Skip Data Points in the Fit.....           | 236 |
|      | Include Derived Parameters.....            | 236 |
| 8.9. | +OTHER Options.....                        | 239 |
|      | <u>Wvl. Range Expansion Fit</u> .....      | 239 |
|      | <u>Try Alternate Models</u> .....          | 239 |
|      | <u>Parameter Uniqueness</u> .....          | 240 |
|      | <u>Simulate Data</u> .....                 | 241 |
|      | Add Opt. Const. to HTML Report.....        | 241 |
|      | <u>Configure Options</u> .....             | 241 |

|           |                                     |            |
|-----------|-------------------------------------|------------|
| <b>9.</b> | <b>Reference - Hardware Tab</b>     | <b>242</b> |
| 9.1.      | Hardware Tab – AlphaSE.....         | 242        |
|           | Hardware .....                      | 242        |
|           | Signal.....                         | 243        |
|           | Calibration .....                   | 244        |
|           | Show Logs .....                     | 244        |
| 9.2.      | Hardware Tab – M-2000 and RC2 ..... | 245        |
|           | Hardware Status .....               | 246        |
|           | System Information .....            | 246        |

|   |            |
|---|------------|
| Controls .....  | 246        |
| <b>10. Reference - Options Tab</b>                      | <b>253</b> |
| 10.1. Display Units.....                                | 253        |
| Wavelength Units.....                                   | 253        |
| Thickness Units .....                                   | 253        |
| Optical Constants .....                                 | 253        |
| ‘Use Defaults’ .....                                    | 254        |
| 10.2. Miscellaneous.....                                | 254        |
| Reset Win. Size .....                                   | 254        |
| Manage Users .....                                      | 254        |
| 10.3. Configuration Controls.....                       | 255        |
| Edit Configuration.....                                 | 255        |
| Import and Save Configuration .....                     | 258        |
| 10.4. About CompleteEASE.....                           | 258        |
| Create Debug File.....                                  | 258        |
| View Error Log .....                                    | 258        |
| <b>11. Appendices</b>                                   | <b>259</b> |
| 11.1. Troubleshooting Guide.....                        | 259        |
| Creating a Debug file.....                              | 259        |
| Reporting Problems to the J. A. Woollam Co. ....        | 259        |
| 11.2. CompleteEASE Data Transfer (to/from WVASE32)..... | 260        |
| Importing CompleteEASE Data to WVASE32: .....           | 260        |
| Exporting WVASE32 Data to CompleteEASE:.....            | 262        |
| 11.3. Contacting the J.A. Woollam Co., Inc.....         | 264        |

# 1. Introduction

Thank you for purchasing a Woollam Spectroscopic Ellipsometer (SE) system. We hope the information contained in this manual will help you develop a better understanding and appreciation for data analysis using the CompleteEASE software.

---

## 1.1. New Features of Interest

CompleteEASE version 4.05 includes many improvements to make this new version easier to use and more powerful. This manual documents all features of version 4.05, but if you are upgrading from an earlier version, you will find the following features of interest.

### Snapshots

A snapshot will compress your data file, model, and fit results into a single file with “ss” extension. Thus, a single snapshot file can be stored or sent and then opened to get back to the same result that you saved. For more details on saving or opening a snapshot, see Section 3.6.

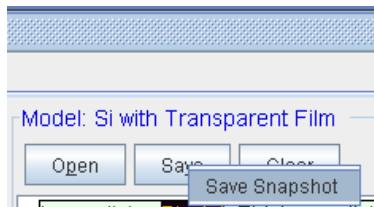


Figure 1-1. Right-click on the Model-Save or Model-Open buttons to Save or Open a Snapshot.

### 3-Deep File Structure

In older versions of CompleteEASE, access was only granted to individual folder “links”. In CompleteEASE 4.05, we have expanded each folder “link” to view 2 sub-levels of folders below the “linked” location. An example of this is shown in Figure 1-2. Here, the only “linked” folder is called Measurements. CompleteEASE automatically shows 2 levels of subdirectories within this folder.

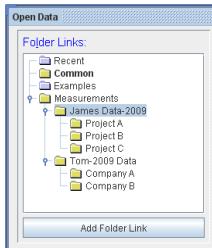


Figure 1-2. CompleteEASE can view and access two levels of sub-directories within the Linked folder.

## Multi-Processor Capability

Due to material and physics limitations the single-core processing performance of current microprocessors is beginning to plateau. Future increases in processing power will come by adding multiple processing cores to the system. This is already beginning; many computers have 2 cores, and in the very near future, all computers will likely have at least 4 (or more) cores.

CompleteEASE has been re-written to take advantage of multi-core capability. For time-consuming operations, CompleteEASE can split the analysis across multiple cores. While performance does not scale linearly with the # of cores, it does improve significantly. During testing of “2 core machines” the performance improvement is  $\approx 1.7x$ . Testing of new computers with 4-core and 8-core processors showed improvements of  $\approx 3.2x$  and  $4.8x$ , respectively.

- OTHER Options  
[Wvl. Range Expansion Fit](#) Increment (eV) = [0.50](#)  
[Try Alternate Models](#)  
[Parameter Uniqueness](#)  
Add Opt. Const. to HTML Report = [OFF](#)  
# of Processor Cores to use (available:8) = [8](#)

Figure 1-3. CompleteEASE can be configured to use processing power from multiple cores.

## Model “roll-back”

Make a mistake and it is now easier than ever to “roll-back” to an earlier point during your analysis session. Rather than relying on a single-step reset, CompleteEASE now keeps track of your model before and after each Fit. The Reset list is cleared each time a new data file is opened.

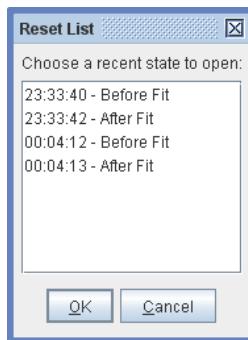


Figure 1-4. Roll-back feature to reset to an earlier point during a single fit session.

## Anisotropic Modeling

The anisotropic modeling capabilities for both Uniaxial and Biaxial materials have been added to CompleteEASE. In fact, with right-click access to convert any layer to its anisotropic equivalent, it is easier than ever to explore the world of anisotropic modeling. For more details, check the Examples of Section 5.5.

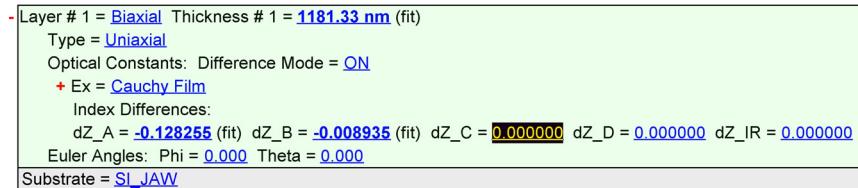


Figure 1-5. Example of an Anisotropic model.

## New Mapping Features

Many advances have taken place in the Mapping section of CompleteEASE. If a camera is available on the system, the camera image can be recorded at each point and then opened with the click of a button on the graph point after the scan. If you are trying to measure small spots at specific locations, the Deskew feature can be very handy. Figure 1-6 shows a typical Scan Pattern Editor screen from CompleteEASE.

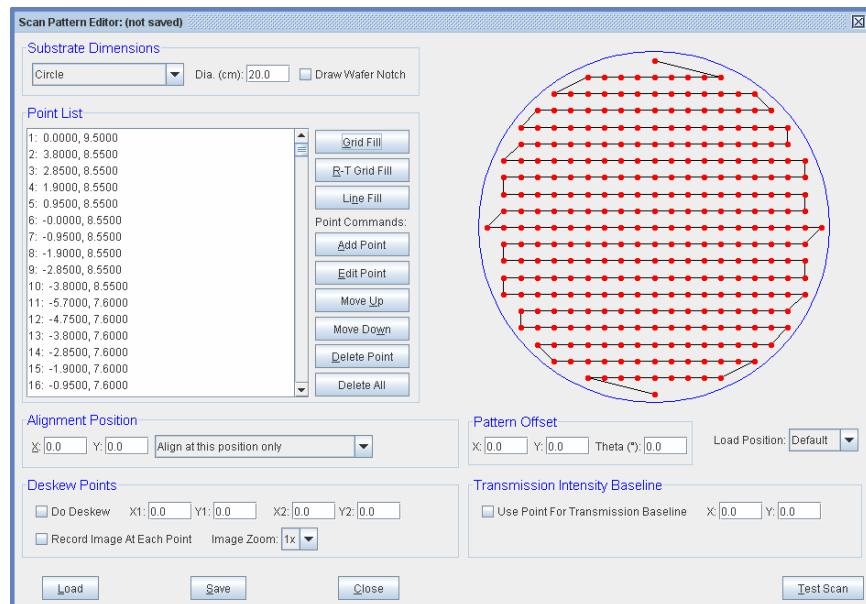


Figure 1-6. Scan Pattern Editor in CompleteEASE

## Easy access to manual

This manual is filled with useful information, so we have made it easier to access in multiple ways. In addition to the printed version shipped with your instrument, you can also find the PDF file for the manual inside the C:/CompleteEASE folder on your computer after installation. In addition, press the F1 key and the manual will appear, as shown in Figure 1-7.

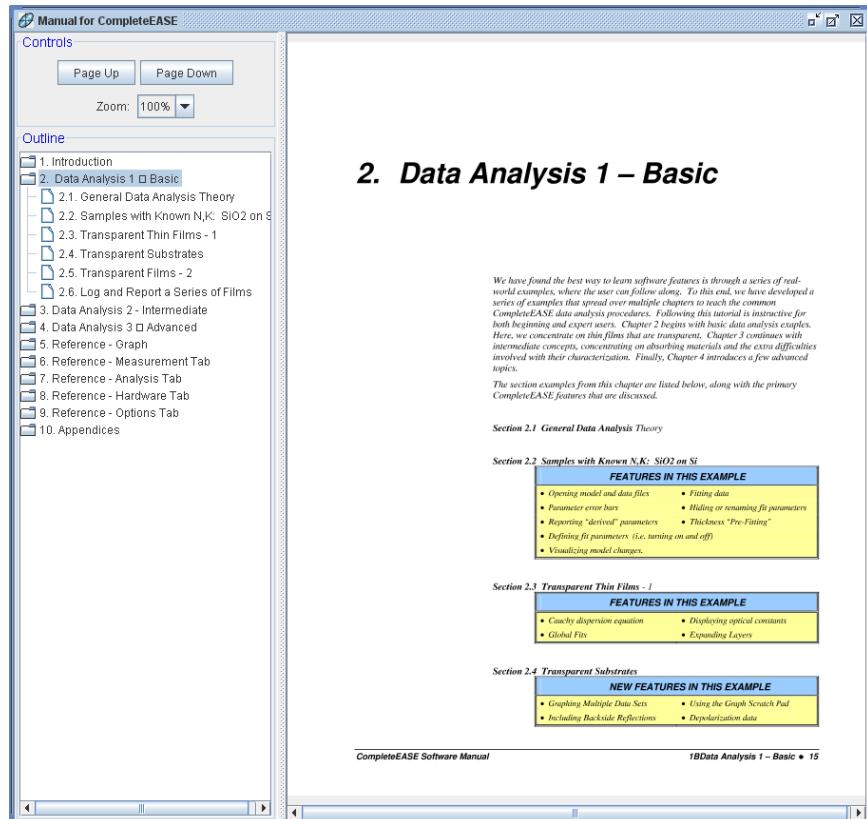


Figure 1-7. Accessible manual from within CompleteEASE.

---

## 1.2. Manual Overview

The organization of the manual is briefly described below.

### **Chapter 1: Introduction**

Chapter 1 will introduce you to ellipsometry. There is good information about basic ellipsometry, along with the installation instructions, a list of short-cut keys, and a list of the “conventions” used throughout this manual. New to this manual, we have added a section regarding “New Features of Interest” as many users are upgrading from earlier versions of CompleteEASE. In addition, new sections on File Structure and User Setup have been added.

### **Chapter 2: Data Collection**

Chapter 2 provides a quick overview of data collection. As the details can vary depending on the instrument and configuration, this chapter is meant only for quick reference and the formal information should be sought from the Hardware manual for your instrument.

### **Chapter 3: Data Analysis 1 – Basic**

There are three chapters devoted to data analysis procedures. Each steps through examples provided with this manual. Chapter 3 describes the basic SE data analysis algorithms used by the CompleteEASE software. All users can benefit from understanding how the most basic models are constructed and operate. Examples in this chapter include:

- Oxides on Silicon
- Transparent Thin Films
- Glass substrate considerations
- Surface Roughness and Index Grading
- Logging and Reporting Results from a Series of Films

### **Chapter 4: Data Analysis 2 - Intermediate**

Chapter 4 continues to build on principles of data analysis, focusing on absorbing materials. The examples are intended to teach the multitude of advanced features within CompleteEASE. Examples in this chapter include:

- Metal Substrates
- Organic monolayers on Gold
- Absorbing Thin Films (B-SPLINE approach)
- Absorbing Thin Films (GENOSC approach)
- Combining SE and Transmission data

## **Chapter 5: Data Analysis 3 – Advanced**

Chapter 5 continues the description of data analysis for advanced applications. Examples in this chapter include:

- Working with Uniformity Maps
- Multi-Sample Analysis
- Model Non-Idealities
- Creating Alloy Files
- Anisotropic Films
- Generalized SE and Mueller-Matrix Analysis

## **Chapters 6 through 10: Feature References**

These chapters are targeted toward advanced users that need an explanation of specific topics. The chapters are organized as follows:

- Chapter 6:** Basic Screen Layout and Graph Panel  
**Chapter 7:** Measurement Tab  
**Chapter 8:** Analysis Tab  
**Chapter 9:** Hardware Tab  
**Chapter 10:** Options Tab

## **Appendices: Additional Information**

The Appendices include additional information for your reference.

- **Appendix 11.1** Trouble-Shooting Guide.
- **Appendix 11.2** Importing/Exporting WVASE32 data files
- **Appendix 11.3** Contacting the J.A. Woollam Company

## 1.3. Installing the Software

### Before Installation

Verify that the computer used to operate the ellipsometer system meets all the requirements listed in Table 1-1. Microsoft Windows XP is the preferred operating system.

Table 1-1. Computer requirements for the CompleteEASE software.

| COMPUTER SPECIFICATIONS | REQUIREMENTS  |
|-------------------------|---|
| Operating System        | Microsoft Windows 98, ME, 2000, XP, Vista                               |
| Memory (RAM)            | 256 MB  |
| Hard Disk Space         | 120 MB  |
| USB Ports               | 1 required, version 1.1 or higher                                       |
| Processor               | Intel Pentium III, AMD Athlon, or higher<br>1 GHz clock speed or faster |
| Display                 | Color display<br>at least 800x600 pixel resolution                      |

*The configuration files are unique for each ellipsometer system. If you have problems with installation, consult the Troubleshooting Guide in Section 11.1*

### Running the SETUP Program

Run the “CompleteEASE\_Setup\_4.00.EXE” application from the provided installation CD. This program is located on the CD along with a folder named “CNF” that contains the configuration files to match one specific ellipsometer system. Setup will install the CompleteEASE program files, the Java Virtual Machine (VM) files which are required to run CompleteEASE, and other related files (material optical constants files, optical model files, example files, etc.). The **CompleteEASE\_Setup** program also installs the calibration and configuration files for your specific instrument from the “CNF” directory.

Follow the onscreen prompts provided by the CompleteEASE\_Setup program. The default directory for installation is **C:\CompleteEASE\**. To minimize compatibility problems, it is recommended to install the software in this directory. This is shown in Figure 1-8. The installation CD includes configuration files for one specific ellipsometer system. If you are installing the CompleteEASE software to run this ellipsometer system, make sure to choose “Full Installation” as shown in Figure 1-9. The CompleteEASE software can be installed on multiple computers for data analysis purposes (most systems include 5-site license). If you are installing software on a computer that will not operate an ellipsometer system, choose “Data Analysis Only”, as shown in Figure 1-9.

**NOTE:** The CompleteEASE software is **only** compatible with the encoded Experimental Data files measured using CompleteEASE. Thus, you can install CompleteEASE at multiple computers, but only for use with data collected by CompleteEASE.

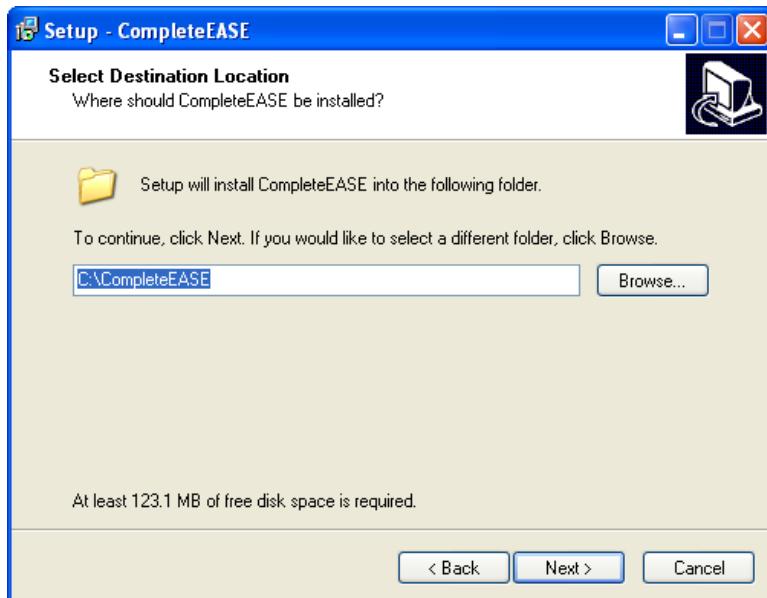


Figure 1-8. Default folder location for CompleteEASE installation.

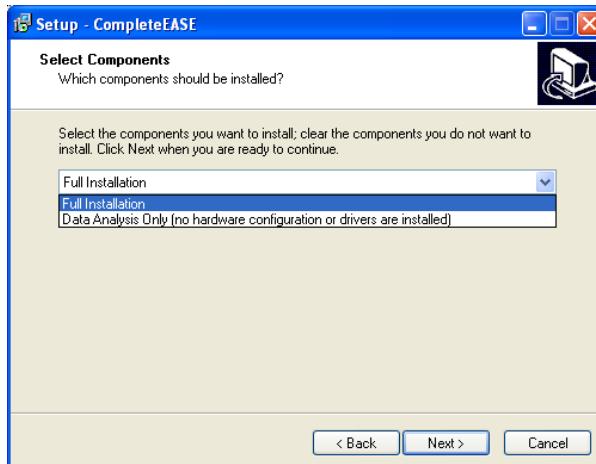


Figure 1-9. CompleteEASE Setup choices. The software can be installed for use with an ellipsometer system or for data analysis only.

The next message you will receive asks which tasks you would like the installation software to perform. The choice ranges from creating icons to associating CompleteEASE file types. These possibilities are shown in Figure 1-10. If you choose, a short-cut icon (Figure 1-11) will be placed on the Windows Desktop to start the CompleteEASE program. However, do **NOT** start CompleteEASE until following the system connection instructions. The software installation process should take less than two minutes on most computers.

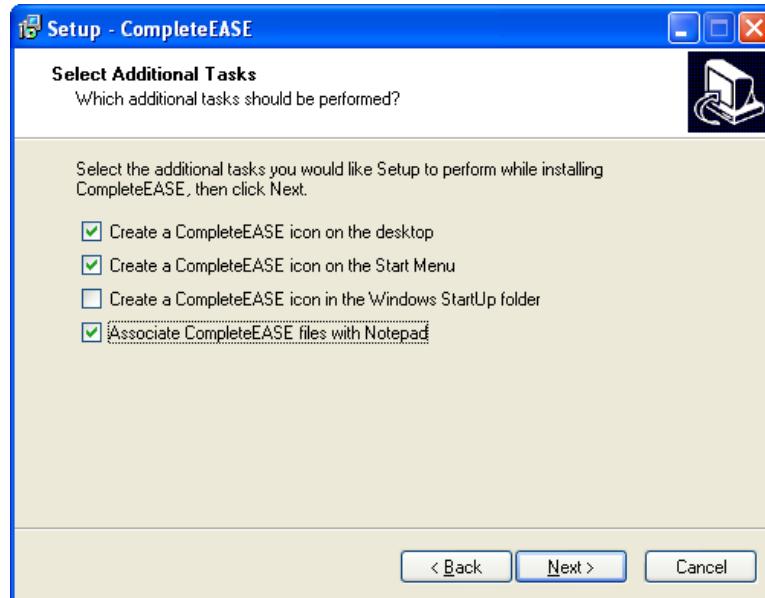


Figure 1-10. Additional Tasks desired during installation of CompleteEASE.

***DO NOT start the  
CompleteEASE  
program at this  
time.***



Figure 1-11. CompleteEASE icon.

## 1.4. Conventions Used in this Manual

The CompleteEASE software is written in JAVA with a Tab-interface to conveniently organize software features. Figure 1-12 shows the front screen of CompleteEASE.

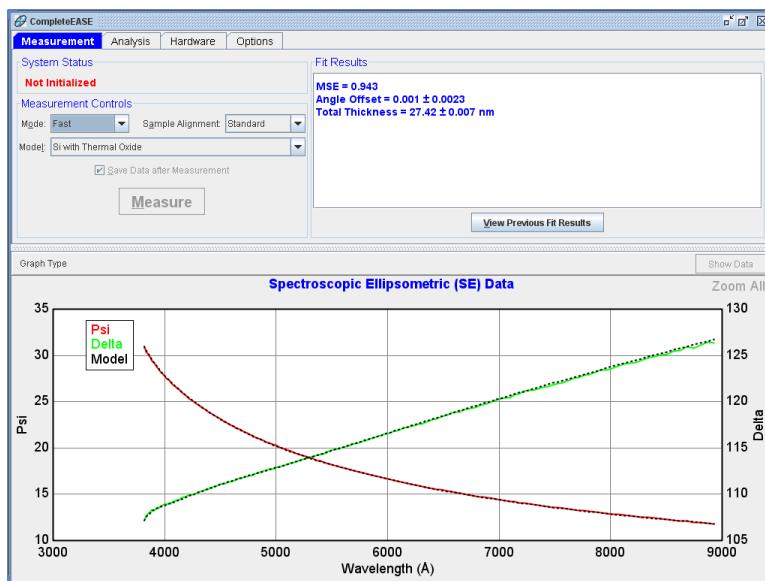


Figure 1-12. CompleteEASE Software

To help the user navigate this manual, the following conventions will be followed to describe features in the CompleteEASE software.

### Tabs

When the software is used with an alpha-SE™ system, there are typically four Tabs, as shown across the top of the software screen: **Measurement**, **Analysis**, **Hardware**, and **Options**. An additional **In Situ** tab is available for M-2000 and RC2 systems that may be applied to real-time measurements. Throughout this manual, Tabs will be written in bold and italics.

### Screen Panels

Within each Tab, there are screen areas referred to as panels. From the **Measurement** tab shown in Figure 1-1, the panels include **System Status**, **Measurement Controls**, and **Fit Results**. Throughout this manual, panels will be written in bold, blue text.

### Buttons

Figure 1-13 shows the **Hardware** tab for CompleteEASE. Notice that there are four panels: **Hardware**, **Signal**, **Calibration**, and **Show Logs**. Within each panel are various buttons. Buttons will be designated with single ‘quote’ marks, such as ‘Re-initialize’ and ‘Park Z-Stage’.

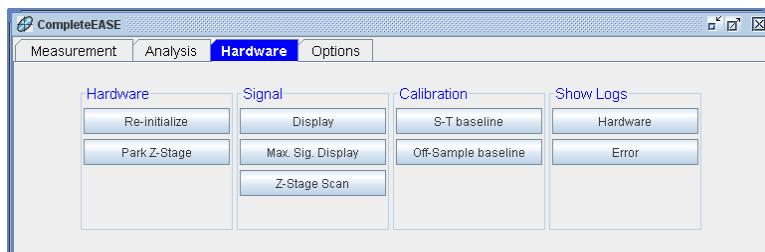


Figure 1-13. **Hardware** Tab, showing Screen Panels and Buttons.

## Model Commands

Figure 1-14 shows the **Analysis** tab. Within the **Analysis** tab, there is a **Model** panel. The model includes many choices – some of which are shown in bold, underlined, red letters. Within this manual, they will also be shown in bold, underlined, red letters. For example, **Add**, **Delete**, and **Save**. Model details are further divided into expandable sections, shown in bold letters preceded by a red + or - symbol. The symbol preceding the text shows whether the section is collapsed (+) or expanded (-). These sections will be listed using bold text with a red + symbol: **+MODEL Options**, **+FIT Options**, and **+OTHER Options**.

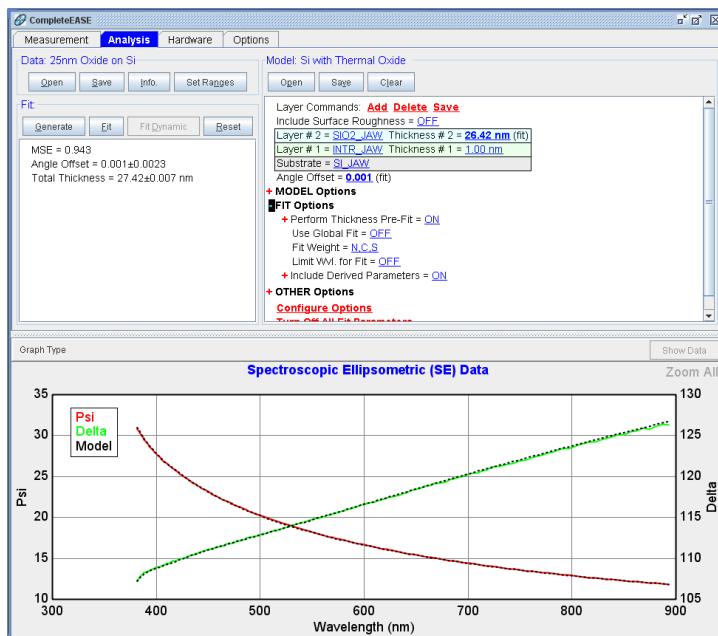


Figure 1-14. **Analysis** Tab showing the Model section.

## Mouse-selected Menus

The CompleteEASE software also utilizes both left- and right- mouse-buttons to access additional menus and features. Throughout this manual, if you need to select the right or left mouse button, you may see the following symbols: (**⌘R**) or (**⌘L**), respectively. Figure 1-15 shows the menu when the right mouse button (**⌘R**) is pressed within the **Fit:** results box.

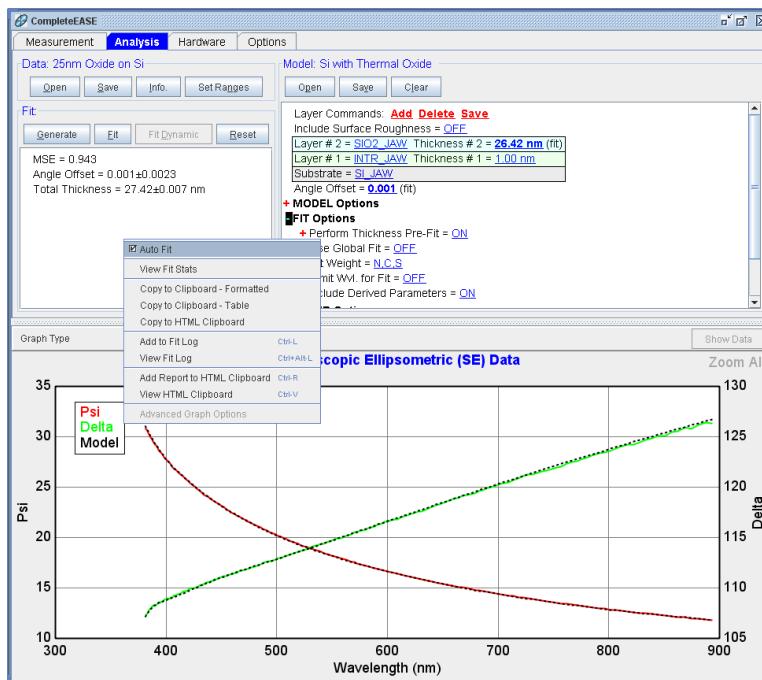


Figure 1-15. Right-clicking mouse ( $\text{Ctrl}+\text{R}$ ) in Fit results section (white area) brings up a special menu related to the Fit.

## Pipelining Descriptions

The descriptions used in above sections can be “pipelined” to form a convenient description of software features or menus. In this case, the description will take on a similar form as:

**Tab>Panel:>‘Button’**

For example, the ‘Open’ button within the **Model:** Panel under the **Analysis** tab is conveniently described as:

**Analysis>Model:>‘Open’**

As another example, the command to right-click the mouse within the **Fit:** Panel from the **Analysis** tab and then choose the “Add to Fit Log” menu choice would read as follows:

**Analysis>Fit:>( $\text{Ctrl}+\text{R}$ )>“Add to Fit Log”**

## 1.5. File Structure

The CompleteEASE software is installed on your hard-drive in a single directory. However, it is helpful to understand the sub-directories used by CompleteEASE. Figure 1-16 shows the sub-directories within the CompleteEASE folder.

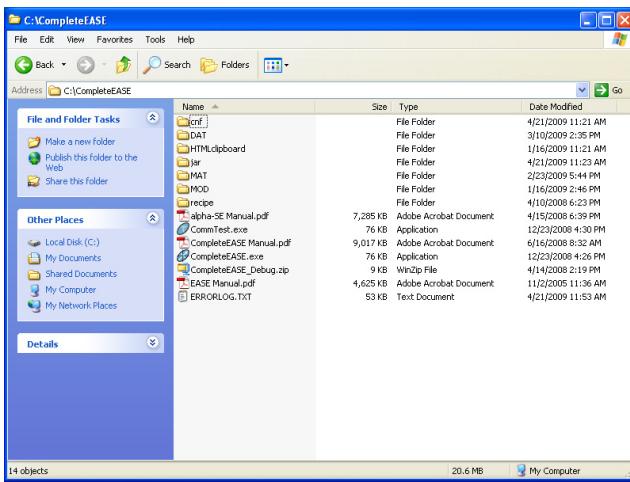


Figure 1-16. Structure within CompleteEASE folder.

The following table provides more details about each of these subdirectories and their function within CompleteEASE.

Table 1-2. Directory Information within CompleteEASE

| DIRECTORY      | FUNCTION   |
|----------------|--|
| cnf            | Hardware configuration files   |
| DAT            | <b>Common</b> Data files, including a sub-folder of Examples that are shipped with the CompleteEASE software. Any data files saved in this directory can be viewed and opened by all users, but are read-only. This directory is not intended for individual user files.             |
| HTML Clipboard | Files and Graphs used by CompleteEASE to construct reports within the HTML Clipboard.  |
| jar            | Java Application files   |
| MAT            | <b>Common</b> Material Files to describe optical constants of materials you may encounter. This folder is further divided into: Advanced, Basic, Dielectric, Metal, and Semiconductor folders. Files within this directory can be viewed and opened by all users, but are read-only. |
| MOD            | <b>Common</b> Model Files to describe a sample and the associated analysis strategy. Further divided into Advanced, Basic, and Calibration Wafers.   |
| Recipe         | <b>Common</b> Recipe Files describe a complete measurement and model strategy. This is pertinent to variable angle or variable measurement point systems and is not used with the alpha-SE system.   |

Although the default directories will always be used by CompleteEASE, the user can create their own directories to store Data files, Models, Materials, and Recipes. To maintain the default files, any sub-directories created within the primary Directories (as listed in Table 1-2) will be treated as “read-only”. For example, the three subdirectories within MOD (Advanced, Basic, and Calibration Wafer) are read-only.

## COMMON Location

Files can also be saved directly within the Mod directory. This location is considered the COMMON directory for Models. Similarly, files located directly in the \DAT or \MAT directory are considered the COMMON locations for Data files and Material files, respectively. To demonstrate this, Figure 1-17 shows the \MOD directory structure, along with a corresponding **Analysis>Model:>‘Open’** dialog box. Notice the same folders are shown in the dialog box, with the addition of “Recent”. Most folders are shown as blue, which represents they are read-only. The only yellow folder is Common as it maintains full access and shows the two files that were directly within the \MOD directory.

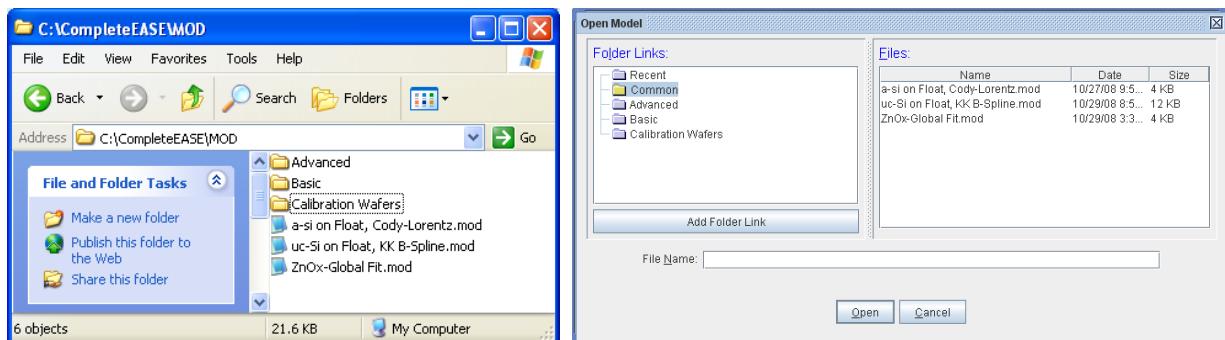


Figure 1-17. Structure within the MOD directory along with the associated Open Model dialog box.

## Folder “Links”

The folders listed for Data, Models, Materials, and Recipes in CompleteEASE are actually “links” to folders on your computer. The actual folders can be located anywhere on the computer. CompleteEASE will retain a list of “links” that you have made to these folders. To view the actual location of a folder, (**Ctrl+R**) on the folder and computer location will show up at the top of the list, as shown in Figure 1-21.

**NOTE:** If the folders on your computer are moved, deleted, or renamed, the “link” inside CompleteEASE will be broken. This can cause unstable behavior and CompleteEASE should be closed and re-opened to re-establish “links” still available.

### Adding Folder “Links” (within CompleteEASE)

It is easy to add “links” to folders on your computer, so they will show up in the CompleteEASE folders list. As an example, we will add a “link” to existing data folder. From the **Analysis** tab, press ‘Open’ from **Data:** and you will see the dialog box as shown in Figure 1-18. The ‘Add Folder Link’ button will allow you to select a folder on your computer to “link” with.

When you press the ‘Add Folder Link’ button, a directory of your computer will appear in the CompleteEASE Folder Browser, as shown in Figure 1-19. If you need to make a new folder, you can press the ‘Create New Folder’ button.

**NOTE:** Before pressing ‘Create New Folder’, you need to position your mouse on the computer location where the new folder is to be created. After pressing the button, verify that the location is correct from the follow-up menu before confirming.

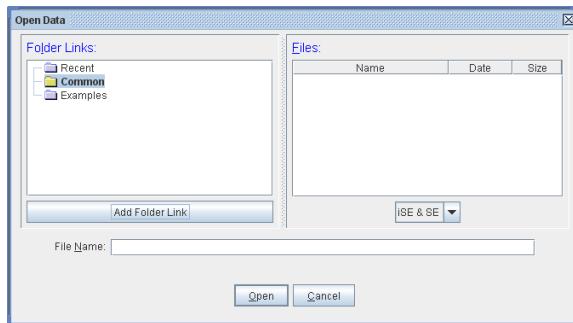


Figure 1-18. Open Data dialog box, showing the **Folder Links:** to data folders on your computer.

As an example, a Folder was created inside C:/Measurements/. First, select this location with your mouse, as shown in Figure 1-19. Next, press the ‘Create New Folder’ button and you will see the Input message, also shown in Figure, to ensure that the location you chose is correct and request the name of new Folder to be created. If the folder location specified is correct, type in a name for the new Folder and press ‘OK’.

**NOTE:** Creating a New Folder as described above does NOT automatically “link” this new folder within CompleteEASE.

After creating the new folder, select this folder from the CompleteEASE Folder Browser list and press ‘Add Folder Link’. The folder will show up in the Open Data window, as shown in Figure 1-20.

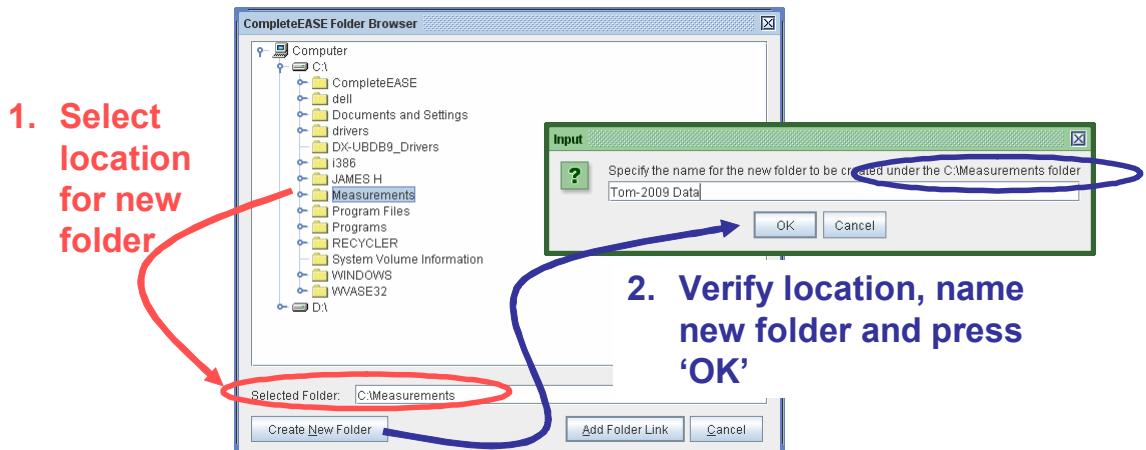


Figure 1-19. CompleteEASE Folder Browser is used to search through folders on your computer. To create a new folder, first select the correct location and then press ‘Create New Folder’ button. Second, type a name for the new folder. It is always wise to verify the location where the new folder will be created on your computer.

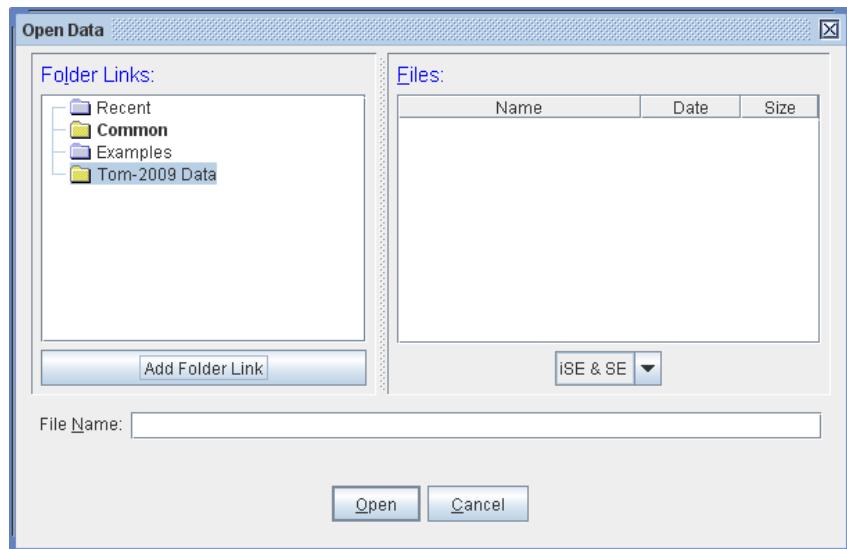


Figure 1-20. Open Data list, showing the new “link” to Tom-2009 Data folder.

### Creating New Sub-Folders

To create a sub-folder within an existing Folder Link, proceed with the new right-click menu option: “Create New Sub Folder”. To do this, press the right-mouse over the Folder location in CompleteEASE, as shown in Figure 1-21, and select “Create New Sub Folder”. Then, type in the name of the new folder you wish to create, as shown to right in Figure 1-21.

NOTE: While the new sub-folder will appear, it is not directly “linked”. The distinction will be further discussed later in this section.

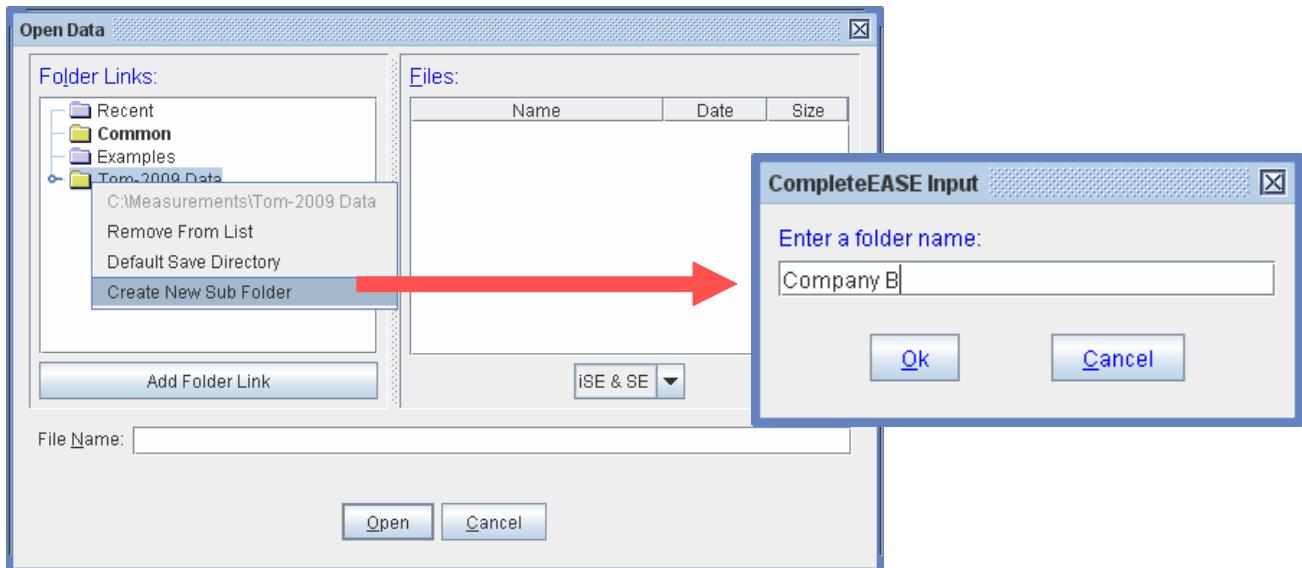


Figure 1-21. Right-click (**Ctrl**) on a folder to access options such as ‘Remove from List’ and ‘Default Save Directory’.

## **Adding Folder “Links” (Drag-and-Drop)**

It is convenient to add new folder “links” to the list shown within CompleteEASE using Windows drag-and-drop features. For example, we may want to store data and results in a separate directory. To demonstrate, a new folder has been created in Windows Explorer at C:\Measurements\James Data-2009\.

To add the “link” to this folder in the CompleteEASE list, choose **Analysis>Data:>‘Open’** to access the dialog box shown in Figure 1-22. Now, switch to Explorer or My Computer within Windows and find the data folder you would like to “link” into CompleteEASE. In this example, the folder is called “James Data-2009”. (**CTRL**) on the folder and hold the mouse button down while you move the folder over to the CompleteEASE Folder area (as shown in Figure 1-22). When you let go of the mouse button, the folder will appear in CompleteEASE. This is not the actual folder, but rather a “link” to the folder location on your computer.

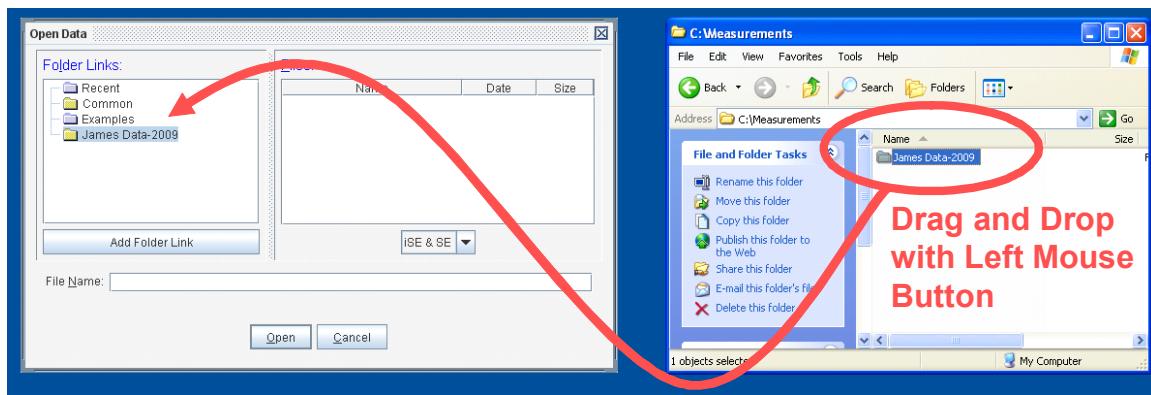


Figure 1-22. Copying folders into CompleteEASE using drag-and drop.

## **Viewing SubFolders**

In older versions of CompleteEASE, access was only granted to individual “links”. In CompleteEASE 4.0, we have expanded each folder “link” to view **2** sub-levels of folders below the “linked” location. An example of this is shown in Figure 1-23. Here, the only “linked” folder is called Measurements. CompleteEASE automatically shows 2 levels of subdirectories within this folder.

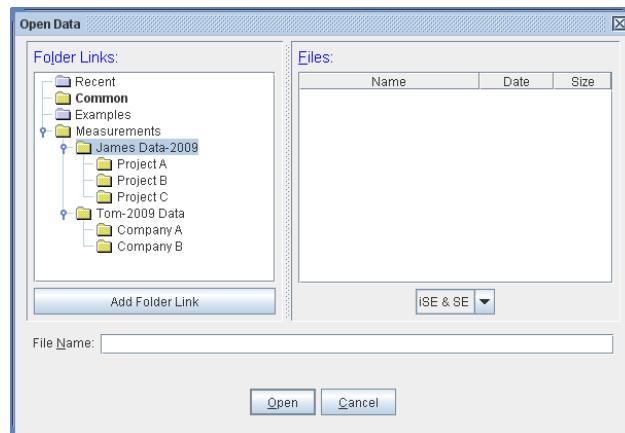


Figure 1-23. Open Data window with a folder called “Measurements” linked. This allows CompleteEASE to view and access two levels of sub-directories within the “Measurements” folder.

CompleteEASE can “link” to any folder on your computer, so you can place the link at different locations to view different levels. You will always view only the 2 sub-levels below the “linked” folders. To demonstrate this, Figure 1-24 shows links to three different folders: “James Data-2009”, “Measurements”, and “Project A”. It turns out that all of these folders are in the same filepath and when expanded, they view the same sub-folders. However, because the “Measurements” link is already 2 levels above “Project A”, it does not expand enough to see the third sub-levels within “Project A”; namely “Run 1”, “Run 2”, and “Run 3”.

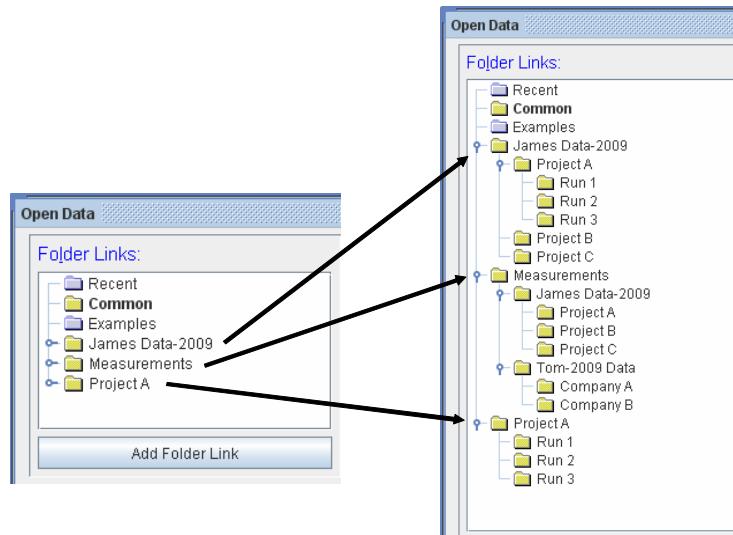


Figure 1-24. Three “links” have been created – pointing to “James Data-2009”, “Measurements”, and “Project A”. Even though these folders are within each other, each will expand to show sub-directories two levels further down.

## Default Save Directory

You can now make any folder the default save directory by ( $\text{Ctrl}+\text{R}$ ) on the folder name as shown in Figure 1-25. The location will be shown in bold text to designate that the default location for opening and saving data files will be located here. Note that the location can be bold in all different locations if this folder is a sub-directory of another link.

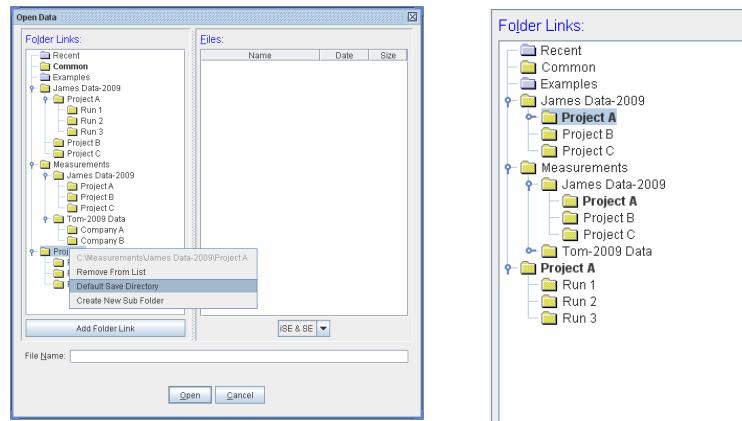


Figure 1-25. ( $\text{Ctrl}+\text{R}$ ) on a folder name and press ‘Default Save Directory’. The location will show up in bold and will become the default location when saving and opening files. Notice, it shows up as bold in all different possible link locations.

## 1.6. Setting Up Multiple Users

A spectroscopic ellipsometer is often used by multiple users. In this case, it is more convenient to allow each user to establish a personal set of folder “links”. However, this requires Login of each user. To configure CompleteEASE for multiple users, make the following changes.

Go to the **Options** tab and select the ‘Edit Configuration’ button. The Configuration Parameters are divided into different areas. Expand the “General” section, as shown in Figure 1-26, and make the following changes:

1. Change “User Log-in Mode” to **Must Log In**.
2. Change “Users Have Own Folders List” to **True**, by selecting the parameter ON check-box.
3. OPTIONAL: You can decide whether to have all CompleteEASE folders visible to all users by changing the “Always Add CE Folder” to **True** or **False**. These are all folders within the CompleteEASE directories on your computer and would show up for all users if this is True.

**NOTE:** After completing these steps, you must restart CompleteEASE before the changes take effect. However, you may also want to setup the User List before restarting (next step).

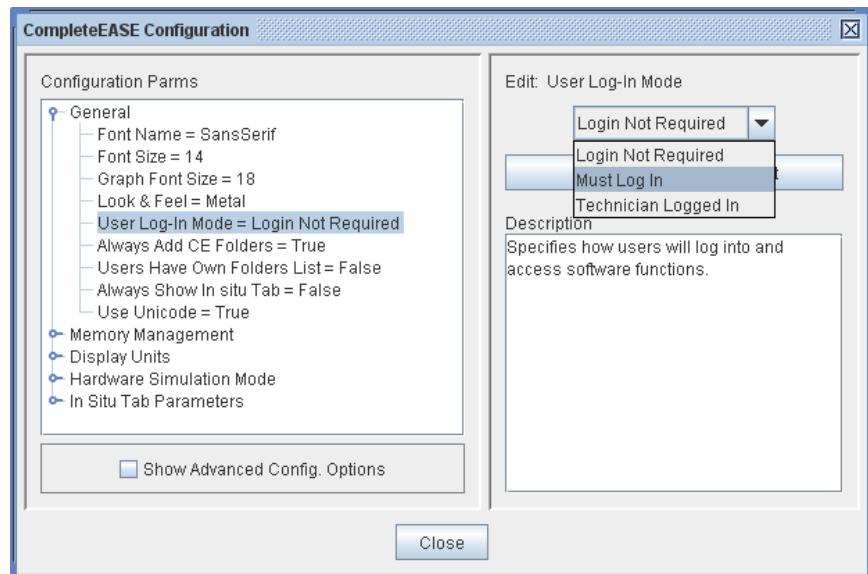
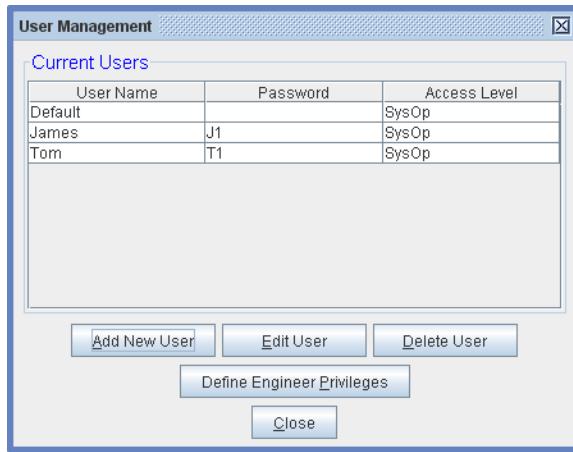


Figure 1-26. CompleteEASE configuration dialog box. The General parameters area has been expanded to view the “User Log-In Mode”, “Always Add CE Folders”, and “Users Have Own Folders List” choices needed to setup multiple users.

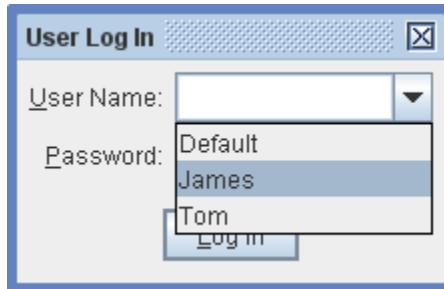
After configuring CompleteEASE for multiple users, you will want to setup each User with their own account. Press **Options>Miscellaneous>‘Manage Users’** and the User Management box will appear, as in Figure 1-27. Press ‘Add New User’ and type in the name and password for each user you wish to add.

**NOTE:** If the password area is left blank, no password will be required to log-in.



*Figure 1-27. Setting up Multiple User Accounts.*

After entering each of the Users with their own account, you should close CompleteEASE and restart. This will allow all of the changes to take effect. When you restart CompleteEASE, it will open by asking to enter your User Name and Password. The user names can be found in the drop-down list, as shown in Figure 1-28.



*Figure 1-28. Log-in is required when multiple users have been setup. The User Names can be selected from a drop-down box.*

Any folders that are added by an individual user at this point will be shown for their account only. However, if the folder is located within the CompleteEASE directory, it will show up for all users. For this reason, it is preferred to create a folder outside of the C:\CompleteEASE directory for files that individual users want to access. For my example, a separate folder has been created at C:\Measurements. Within this folder, each user has their own sub-directory and CompleteEASE can be configured by each user to link to only the folders they need to view.

## 1.7. Short-cut Guide

There are two types of short-cuts within CompleteEASE. First, like with all software, if a letter is shown that is underlined, the short-cut for that command is to hold ALT button and press that letter. For additional short cuts that are more global, incorporate the CTRL, SHIFT, and ALT buttons. These additional short cuts are listed in Table 1-3.

Table 1-3. Short-cut reference.

| SHORT CUT               | FUNCTION   |
|-------------------------|--|
| CTRL-M                  | Go to <b>Measurement</b> Tab   |
| CTRL-A                  | Go to <b>Analysis</b> Tab  |
| CTRL-H                  | Go to <b>Hardware</b> Tab  |
| CTRL-O                  | Go to <b>Options</b> Tab   |
| CTRL-P                  | Graph the Psi data curves  |
| CTRL-D                  | Graph the Delta data curves  |
| CTRL-N                  | Graph the “N” data curves (N,C,S format)   |
| CTRL-C                  | Graph the “C” data curves (N,C,S format)   |
| CTRL-S                  | Graph the “S” data curves (N,C,S format)   |
| CTRL-1                  | Graph the <e1> data curves   |
| CTRL-2                  | Graph the <e2> data curves   |
| CTRL-T                  | Graph the Intensity data   |
| CTRL-Z                  | Graph the Depolarization data  |
| CTRL-SPACE BAR          | Switch view from single-point to Map/Dynamic                                       |
| CTRL-L                  | Add to Fit Log   |
| CTRL-ALT-L              | View Fit Log   |
| CTRL-R                  | Add Report to HTML Clipboard   |
| CTRL-V                  | View HTML Clipboard  |
| CTRL-ALT-O              | Toggle Default Optical Constant units between “e1 & e2” and “n & k”                |
| CTRL-ALT-W              | Toggle Default wavelength units between “nm” and “eV”                              |
| CTRL-ALT-S              | Show graph statistics  |
| CTRL-ALT-SHIFT-I        | Add the <b>In Situ</b> Tab   |
| SHIFT-Mouse roller      | When positioned over model parameter, it will increase or decrease this parameter. |
| CTRL-SHIFT-Mouse roller | Same as SHIFT-Mouse roller, but with smaller parameter increments.                 |

If you are working with Uniformity Mapping data, the following short-cuts can help manipulate the data and graphs.

*Table 1-4. Short-cut reference for mapping data.*

| SHORT CUT                     | FUNCTION   |
|-------------------------------|--|
| CTRL-Click on Point           | Select/De-Select Point                           |
| CTRL-ALT-Click on Point       | Delete Point                                     |
| CTRL-ALT-SHIFT Click on Point | Show camera image from point<br>(when available) |
| CTRL-SPACE Bar                | Switch view from single-point to Map             |

## 1.8. What is Spectroscopic Ellipsometry?

Ellipsometry is a non-destructive optical technique in which the sample to be characterized is illuminated with a beam of polarized light, as shown in Figure 1-29. Ellipsometry measures the change in polarization state of the measurement beam induced by reflection from (or transmission through) the sample. The change in polarization state is commonly characterized by the ellipsometric Psi ( $\Psi$ ) and Delta ( $\Delta$ ) parameters defined in Eqn. (1-1):

$$\tan(\Psi) \cdot e^{i\Delta} = \rho = \frac{r_p}{r_s} \quad (1-1)$$

In this equation, rho ( $\rho$ ) is defined as the ratio of the reflectivity for p-polarized light ( $r_p$ ) divided by the reflectivity for s-polarized light ( $r_s$ ).  $\rho$  is a complex number, and the ellipsometric parameters simply report this value in polar form:  $\tan(\Psi)$  is the magnitude of the reflectivity ratio, and  $\Delta$  is the phase. Ellipsometry offers three main advantages over simple intensity-based reflection or transmission measurements:

1. **Precision** As the change in polarization state is defined by a ratio, ellipsometry is not sensitive to changes in the absolute intensity of the measurement beam (i.e., the sample itself is the ‘reference’ for the measurement). Thus, it can remain accurate without knowing “absolute” intensity values.
2. **Sensitivity** The phase information contained in the ellipsometric  $\Delta$  parameter provides enhanced sensitivity to ultra thin films, even down to the sub-nm thickness level.
3. **Information** Ellipsometry measures 2 values (Psi and Delta) at each wavelength, doubling the information content compared to an intensity reflection or transmission measurement.

The high accuracy, precision, and sensitivity of the ellipsometric measurement make it highly suited for demanding thin film metrology applications.

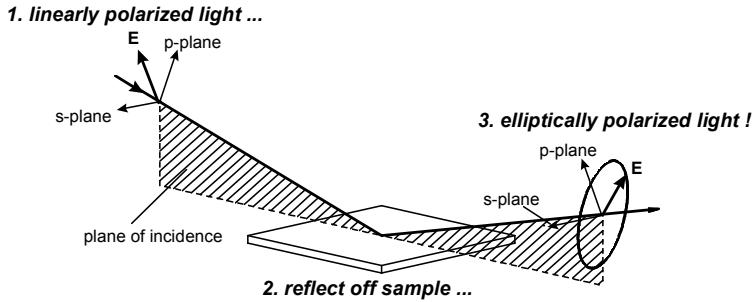


Figure 1-29. Interaction of polarized light with a sample.

In Spectroscopic Ellipsometry (SE), Psi and Delta values are acquired as a function of wavelength. This greatly increases the information content in the data set, enabling the simultaneous determination of multiple sample properties. However, to extract sample parameters such as film thickness and optical constants from the measured SE data set, an optical model must be built to fit the data. The CompleteEASE software provides a graphical user interface for building models and displaying measured data and model fits. The fundamentals and theory of data analysis is explained in more detail in Section 3.1. The CompleteEASE program also provides a simple interface to the SE hardware, making acquisition of accurate SE data fast and easy.

For more information on ellipsometry theory, see the following references:

1. H. Tompkins and E. Irene, eds. [Handbook of Ellipsometry](#), William Andrew Publishing, New York, 2005.
2. H. Fujiwara, [Spectroscopic Ellipsometry Principles and Applications](#) John Wiley & Sons, West Sussex, England 2007.
3. J.N. Hilfiker and J.A. Woollam, [Ellipsometry](#), in [Encyclopedia of Modern Optics](#), edited by Robert D. Guenther, Duncan G. Steel and Leopold Bayvel, Elsevier, Oxford, 2004.
4. J. A. Woollam et al., “Overview of Variable Angle Spectroscopic Ellipsometry (VASE), Part I: Basic Theory and Typical Applications”, [SPIE Proc. CR72](#) (1999) 3.
5. B. Johs et al., “Overview of Variable Angle Spectroscopic Ellipsometry (VASE), Part II: Advanced Applications”, [SPIE Proc. CR72](#) (1999) 29.
6. H.G. Tompkins and W.A. McGahan, [Spectroscopic Ellipsometry and Reflectometry](#), John Wiley & Sons, 1999.
7. R.M.A. Azzam, and N.M. Bashara, [Ellipsometry and Polarized Light](#), North Holland Press, Amsterdam 1977, Second edition 1987.

# 2. Data Collection

The first step to any ellipsometry measurement is collection of data with the ellipsometer. These operations are better discussed in the hardware manual for each instrument. CompleteEASE is used with alpha-SE, M-2000, RC2, and AccuMap-SE ellipsometers from the Woollam Company. The details for data collection depend on both the system and individual ellipsometer configuration. This chapter provides a basic overview of CompleteEASE data collection.

**NOTE:** Instructions in this chapter are representative of various systems. For more complete instructions, including details on system alignment and calibration, please consult your corresponding Hardware manual.

## 2.1. alpha-SE Systems

CompleteEASE uses a simplified screen for data collection with the alpha-SE, as there is only one angle of incidence and no mapping to consider. The Measurement tab for an alpha-SE will appear as in Figure 2-1.

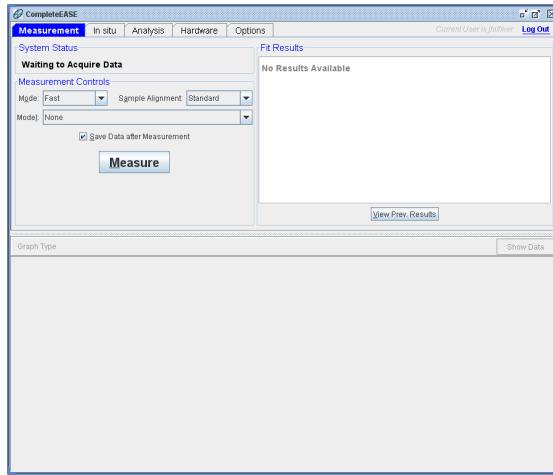


Figure 2-1. Measurement tab for alpha-SE systems.

There are four choices to make before collecting data. These are the measurement “Mode”, the type of “Sample Alignment”, the “Model” to use for data analysis, and whether to “Save Data after Measurement”. The first three options provide a drop-down menu, as shown in Figure 2-2. Table 2-1 describes each choice in more detail.

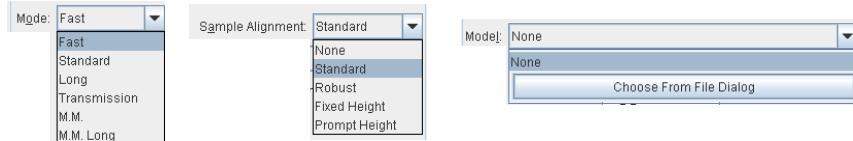


Figure 2-2. Options for measurement Mode, Sample Alignment, and Model.

Table 2-1. Measurement Settings for an alpha-SE.

| Category         | Option  | Description   |
|------------------|---|---|
| Mode             | Standard<br>Fast<br>Long<br>Transmission<br>M.M.<br>M.M. Long | Use for most measurements (~ 10 seconds)<br>Quick measurements (~ 3 seconds)<br>Low reflectivity samples or high precision measurements (~30 seconds)<br>Collects Intensity Transmission measurements.<br>Mueller-matrix measurement – for anisotropic and depolarizing samples<br>High Accuracy Mueller-matrix measurement   |
| Sample Alignment | None<br>Standard<br>Robust<br>Fixed Height<br>Prompt Height   | Stage location is below beam for straight-through (90°) measurements.<br>Use for standard reflected measurements. This setting does a quicker search for the light beam near the previous alignment position.<br>A thorough alignment of the light beam that searches over the full translation range. Use for glass substrates with multiple reflected beams.<br>Moves sample stage to height described in hardware configuration file.<br>Allows user to enter the sample stage height for measurement. It is often helpful to first perform a z-stage scan from the <b>Hardware</b> tab. |
| Model            |   | Press “Choose from File Dialog.”<br>All default models are saved within various folders including:<br><i>Common, Advanced, Basic, and Calibration Wafers</i><br>Only models in the COMMON folder will appear in the drop-down list.   |

## Common Models

For convenience, you can move Models that are commonly encountered into the “Common” folder. To move into the Common folder location, go to the **Analysis** tab and press ‘Open’ from the **Model:** section. Search for the model of interest and then drag the model name (right side of Figure 2-3) with mouse to the Common folder (left of Figure 2-3). You can do this with multiple models.

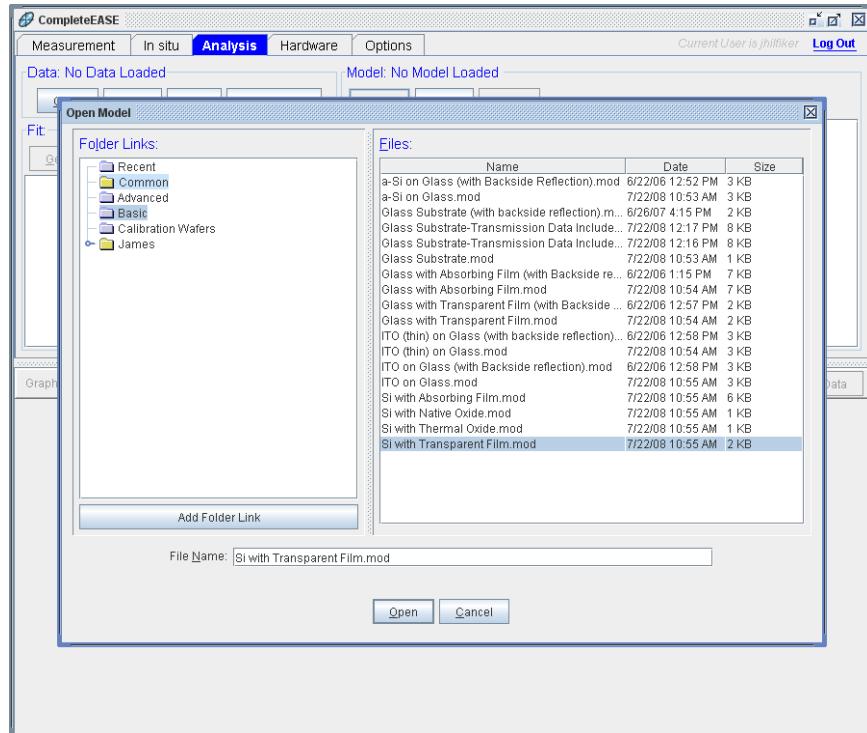


Figure 2-3. From the **Analysis** tab, press ‘Open Model’ and then you can drag-and-drop models from any folder (listed on right) into the Common folder (shown on left).

All models that you move to the Common folder will now appear in the drop-down menu from the **Measurement>Measurement Controls>Model** drop-down menu. This is shown in Figure 2-4, where the Common folder (left) has two models and these same models appear in the Model drop-down menu (right).

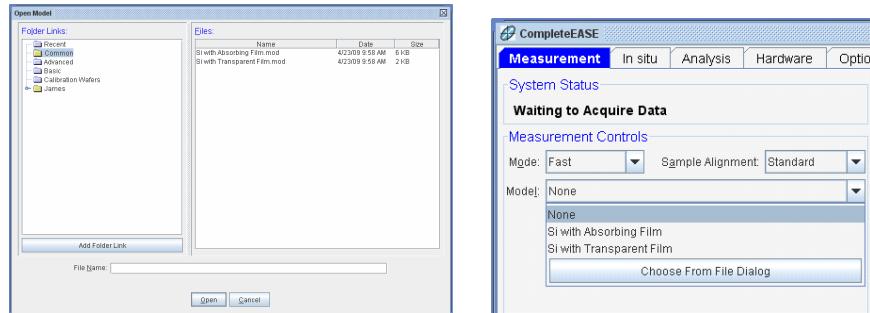


Figure 2-4. The models moved to the Common folder (shown on left) will be quickly accessible from the **Measurement** tab pull-down Model menu (seen on right).

## Measuring a Sample

Once the Mode, Sample Alignment, and Model are selected, you can press the ‘Measure’ button to begin the measurement, as seen in Figure 2-5. As the alpha-SE has automated sample alignment, the system will align to the sample (using the selected Sample Alignment) and then collect measured data (using the selected Mode). Finally, if a Model was selected, the data will be analyzed to determine the resulting film properties.

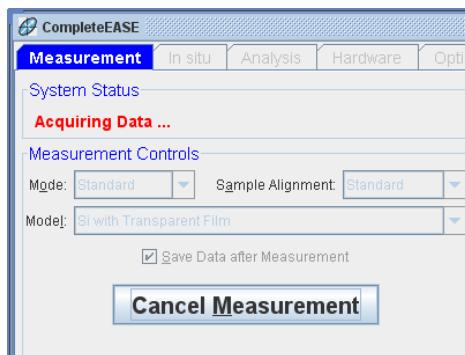


Figure 2-5. Pressing ‘Measure’ will start the data collection procedure. The **System Status** will be updated to show the current hardware operation.

If the “Save Data After Measurement” check-box was selected, a dialog box will appear, as shown in Figure 2-6. Find the location you wish to save the file within the **Folder Links:** area and type in a File Name and Comment. If the folder “link” does not exist, you can create a new folder or add a new link. These instructions were detailed in Section 1.5.

**NOTE:** CompleteEASE data files are encrypted & saved with “.SE” or “.jSE” extensions. These files are only accessible by the CompleteEASE program.

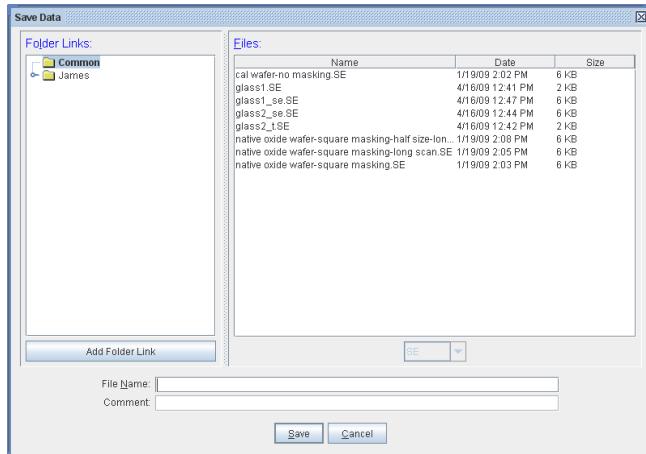


Figure 2-6. Save Data dialog box. Type a File Name and comment and then press ‘Save’.

After SE data is acquired, the model analysis will be performed and the fit parameters displayed in the Fit Results panel. The model fit to the measured data is also displayed in the graph: the black dashed “Model” curves should lie essentially on top of the colored Psi and Delta measured data curves if the model fits the data well. If this is not the case, the wrong model was selected to analyze the data. The final result for a thin oxide on Silicon is shown in Figure 2-7. The model parameters will be reported in the **Measurement>Fit Results** section, while a graph of Psi and Delta versus wavelength are displayed at the bottom of CompleteEASE – along with corresponding Fit curves from the model.

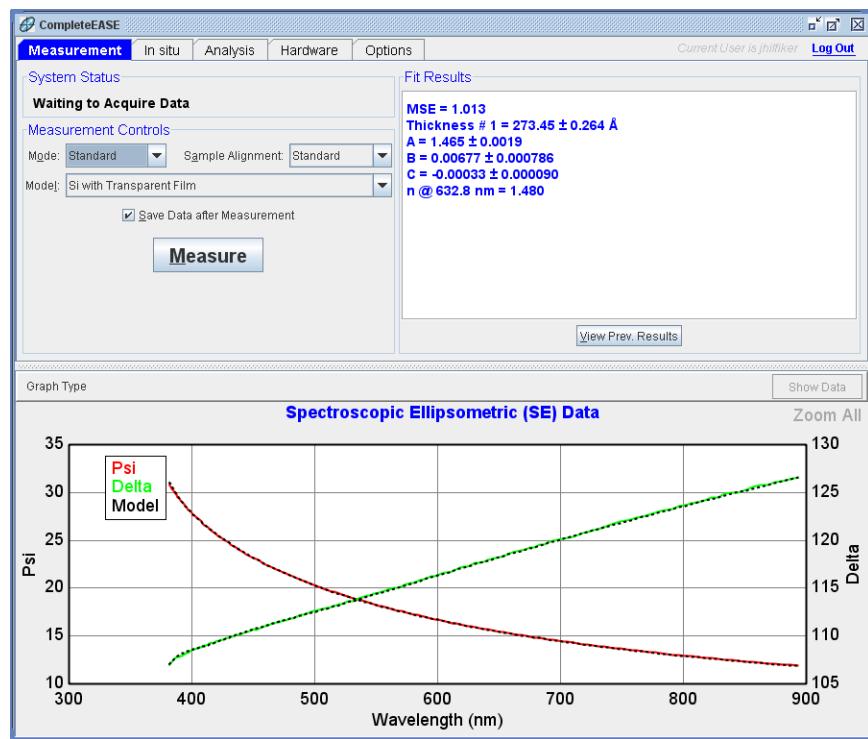


Figure 2-7. Successful measurement of thin dielectric film using an alpha-SE system.

## 2.2. M-2000, RC2, and AccuMap-SE Systems

For M-2000, RC2 and AccuMap-SE systems, there are more data collection choices. This chapter will discuss the basic options for typical systems. As there are many different configurations, it is suggested you consult your Hardware manual for the details of your system and configuration. Figure 2-8 shows a representative CompleteEASE **Measurement** tab for an M-2000 with mapping and camera. Due to the number of choices for any measurement (how to measure, where to measure, etc.), CompleteEASE uses a Recipe to describe all details. These recipe files can be created and saved for any specific measurement or sample type.

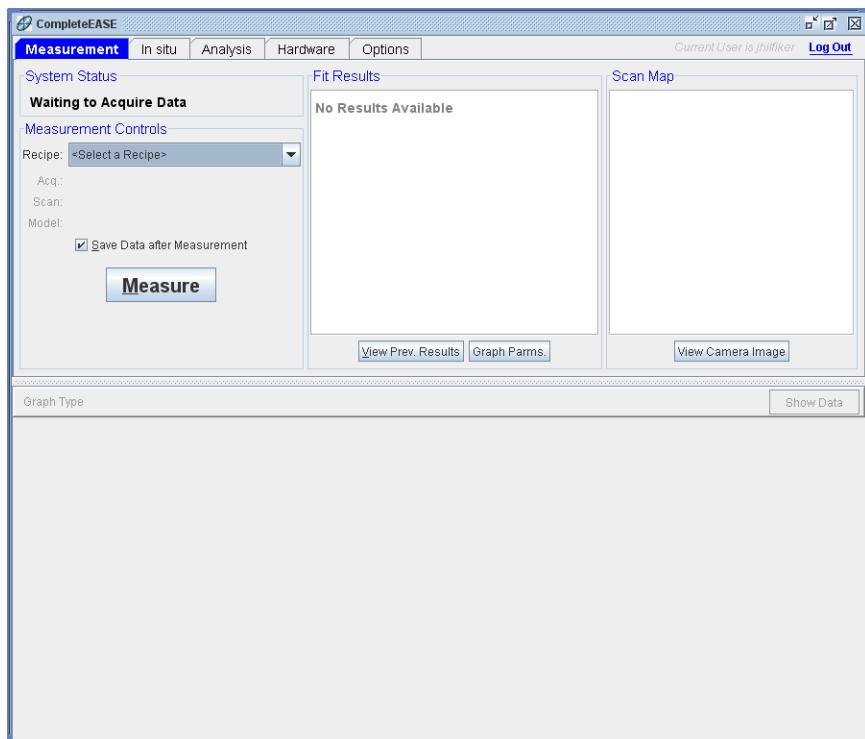


Figure 2-8. Measurement tab for an M-2000 system with automated angle of incidence, automated sample alignment, automated sample translation, focusing optics, and an integrated camera.

### Measurement Recipe

The measurement controls for this type of system are integrated into a Recipe. Each Recipe describes the three basic components of data collection: 1) Data Acquisition, 2) Mapping Scan settings, and 3) Modeling.

The drop-down box from **Measurement>Measurement Controls>Recipe:** allow the following options: 1) Prompt for Acquisition Parameters, 2) Prompt for Recipe Components, 3) list of all Common recipes, 4) Choose From File Dialog, and 5) Create/Edit Recipe. These options are shown in Figure 2-9.

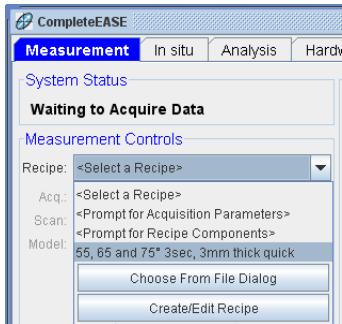


Figure 2-9. Recipe Options.

### **<Select a Recipe>**

This listing is not an option, but rather a note to the user that they need to Select a Recipe or change this setting before they can proceed.

### **<Prompt for Acquisition Parameters>**

This option will by-pass the Scan Pattern and Model, assuming you only want to measure at a single point and save data for modeling at a later time. You will be allowed to specify the Data Acquisition Parameters, from a box similar to shown in Figure 2-10. The options listed in the Acquisition Parameters box are described in Section 2.3.

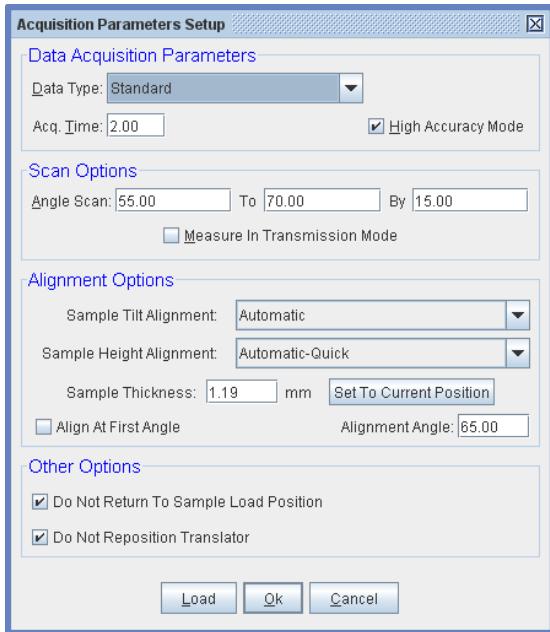


Figure 2-10. Acquisition Parameters Setup dialog box.

### **<Prompt for Recipe Components>**

This option allows the user to select the individual recipe components, which include Acquisition Parameters, Scan Pattern, and Model – as shown in Figure 2-11. If the recipe components are not established, they can also be created from the Recipe Components dialog box.

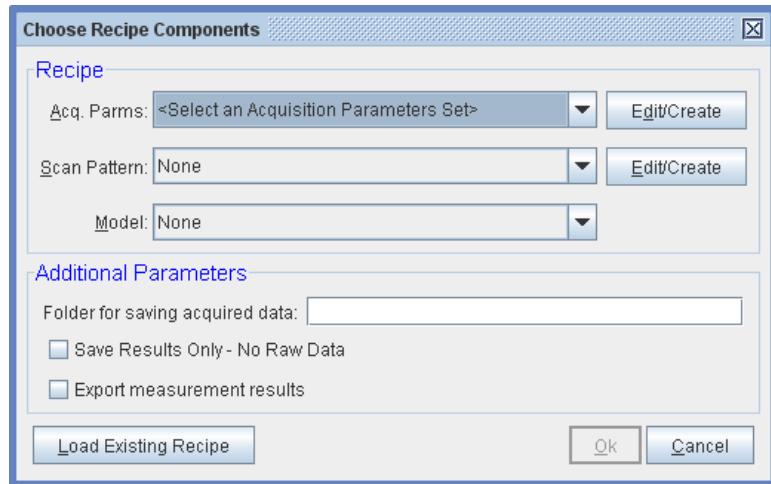


Figure 2-11. Choosing the various components for a Recipe.

### Common Recipes

All recipes that are saved in the Common Folder (C:\CompleteEASE\recipes) will appear in the drop-down list as shown in Figure 2-9. In this example, the Recipe called “55, 65, and 75° 3sec, 3mm thick quick” was created and moved to the Common Folder. To move a recipe to the Common Folder, select the ‘Choose From File Dialog’ option that is described next. This will open the Recipe Dialog box, as shown in Figure 2-12. Navigate through the folder “links” on left to find the recipe you would like to add to Common folder. Then, drag-and-drop the recipe listed under **Files:** to the Common folder listed under **Folder Links:**.

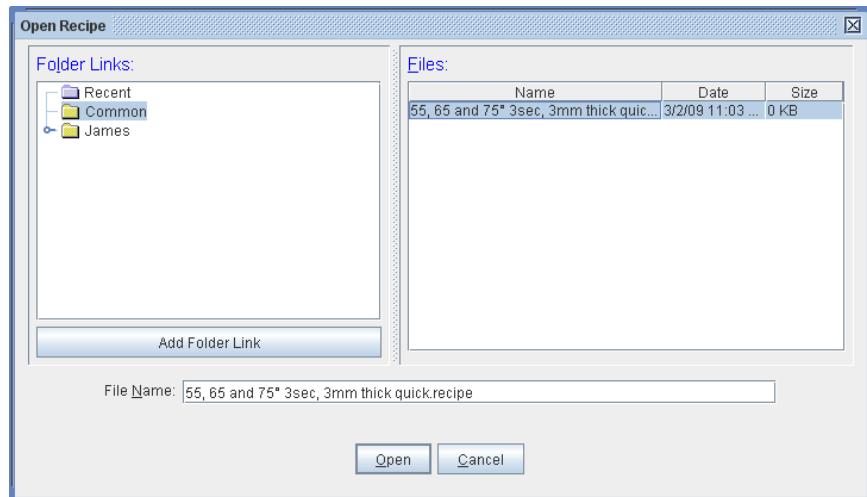


Figure 2-12. Open Recipe dialog box.

### ‘Choose From File Dialog’

This button opens a window to view the Folder links on your computer that may contain recipes, as shown in Figure 2-12. Navigate to find the desired recipe and select it to open.

### **'Create/Edit Recipe'**

The final button allows you to create or edit a recipe. This selection opens the same box as shown in Figure 2-11. Each of the options for a recipe will be described later in this chapter.

The three primary components of any recipe are the Acquisition Parameters, Scan Pattern, and Model; as shown in Figure 2-13. Each of these components is discussed in further detail.

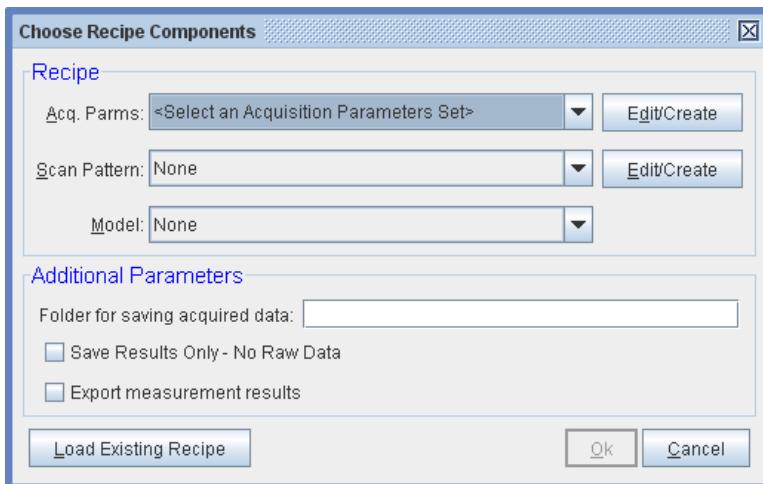


Figure 2-13. Components of a Recipe.

## 2.3. Acquisition Parameters

The Acquisition Parameters describe how the data will be collected at each point of a Measurement Recipe (whether single-point or scan). A common box for Acquisition Parameter choices is shown in Figure 2-14.

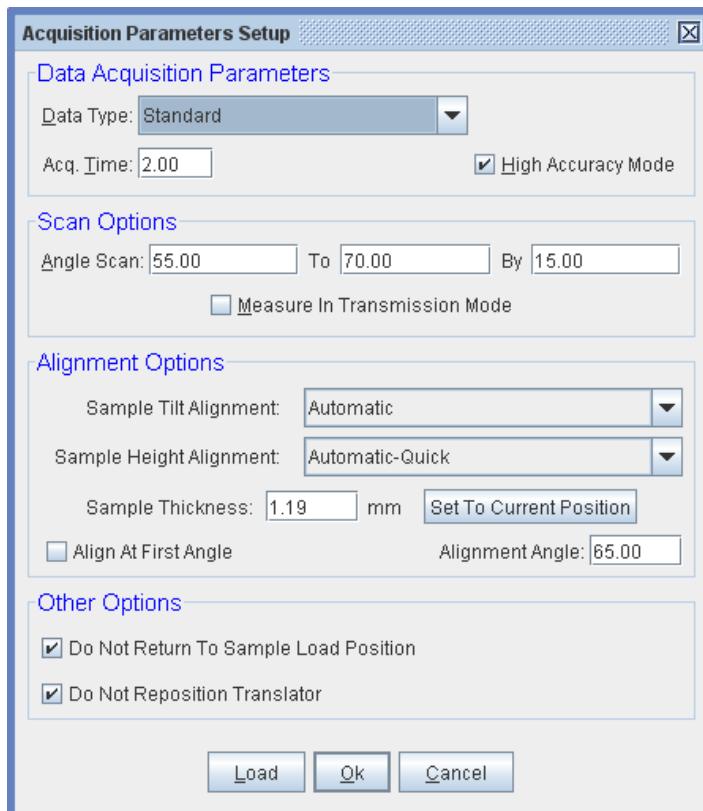


Figure 2-14. Acquisition Parameters Setup for M-2000 and RC2 systems. Choices listed above can vary from system-to-system.

### Data Type

The Data Type specifies the type of data to collect during the measurement, as shown in Figure 2-15.

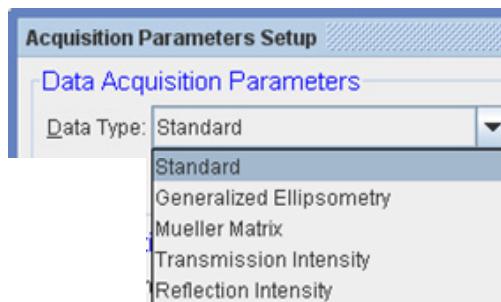


Figure 2-15. Different Options for Data Type.

## **Standard**

Most applications require a “Standard” measurement. This is simply a standard Spectroscopic Ellipsometry measurement. The data collected will include Psi and Delta versus wavelength and angle of incidence. In addition, the depolarization and intensity reflected will be measured. However, the measurement accuracy of reflected intensity and depolarization depends on the accuracy of recent intensity baselines and DC calibrations, respectively. For more details, please consult your Hardware manual. Most models will ignore the depolarization and Intensity measurements, unless instructed to consider this *extra* data.

## **Generalized Ellipsometry**

Measurement of the complete Jones matrix of a sample, including the off-diagonal elements (which are assumed equal to zero for Standard SE measurements). This type of measurement is useful for anisotropic samples where the optical axis is not aligned parallel or perpendicular to the plane of incidence. Generalized Ellipsometry measurements are not compatible with measurements that exhibit depolarization, as it is based on a Jones matrix description of the interaction between measurement beam and sample.

Generalized Ellipsometry measurements consist of three ratios, so you will end up with three Psi curves and three Delta curves for each angle of incidence that is measured.

## **Mueller Matrix**

Measurement of the polarization change using Stokes vectors to describe the light beam. The Mueller-matrix is a 4 X 4 matrix, but not all elements can be measured with each ellipsometer. In fact, the only ellipsometer to measure all 16 elements of the Mueller-matrix is the RC2 system. For most samples, there is significant redundancy in the Mueller-matrix and no need to measure all 16 elements. For isotropic samples (with or without depolarization), the complete interaction can be described by measuring 4 elements (M11, M21 or M12, M33 or M44, and M34 or M43). If the sample also contains anisotropy, the number of necessary elements climbs to 7 or 8. Only for the most advanced samples are more elements required for complete characterization. Thus, less than 1% of all Ellipsometry Applications require Mueller-matrix measurements.

## **Transmission Intensity**

Measure Intensity of transmitted light through the sample.

## **Reflection Intensity**

Measure Intensity of reflected light .

## **Sample Alignment**

Sample Alignment options depend on the type of system and configuration. In general, there are two basic steps to sample alignment: Tilt alignment and Height alignment. Common selection for each are described in this section.

## Tilt Alignment

Tilt alignment refers to the tip and tilt of sample relative to the incoming light beam such that the reflected beam is aligned on the receiver unit at the correct angle of incidence. Tilt alignment options include Skip, Manual, or Automated; as shown in Figure 2-16.

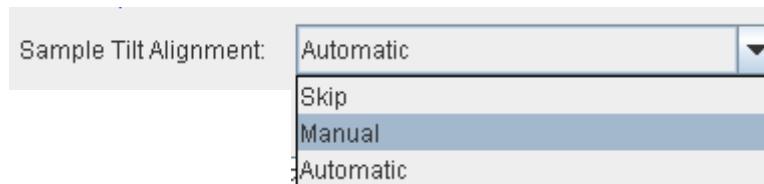


Figure 2-16. Options for Sample Tilt Alignment.

The Tilt alignment is often Skipped when using focusing probes, as the tip-tilt alignment becomes less sensitive. It can also be skipped for applications where common samples are measured that remain flat. For example, if a system is continuously used to measure 200mm silicon wafers, the tip-tilt alignment of each wafer will probably be very similar from sample-to-sample.

For Manual or Automatic Alignment, the system will study the reflection of a light beam off the sample that is incident on a 4-quadrant detector. This detector allows the beam to be centered onto the 4-detector elements by adjusting tip and tilt until all 4 detectors have the same intensity. This method allows very repeatable alignment of the beam from sample-to-sample. An example of the Tilt Alignment step for an Automatic System is shown in Figure 2-17.

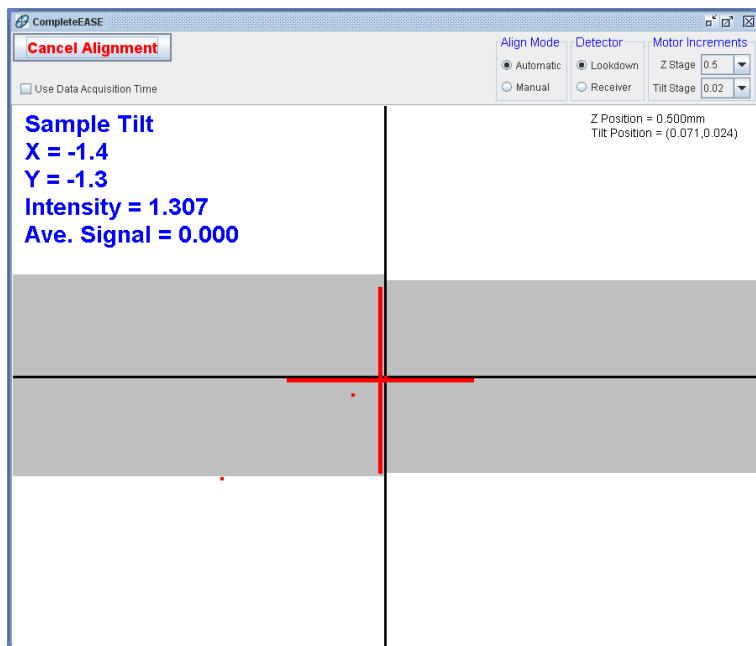


Figure 2-17. Sample Tilt Alignment Window.

## Sample Height Alignment

Sample Height Alignment refers to the adjustment of ellipsometer beam relative to the surface of a sample to ensure correct positioning and adjustment for samples of different thickness. This adjustment becomes increasingly important for systems with smaller spot size (like Focusing ellipsometers). It is also more important to test the Sample Height Alignment when many samples of different thickness will be tested on the same Ellipsometer. The common choices for Sample Height Alignment are shown in Figure 2-18. For Automated Height Alignment, the reflected beam is detected by the Receiver unit and the intensity is recorded versus different Z-Height positions. This is demonstrated in Figure 2-19. The position of highest intensity is assumed to be the correct Z-Height for alignment of the sample.

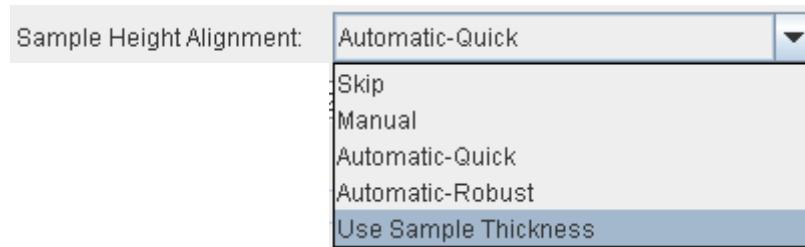


Figure 2-18. Options for Sample Height Alignment.

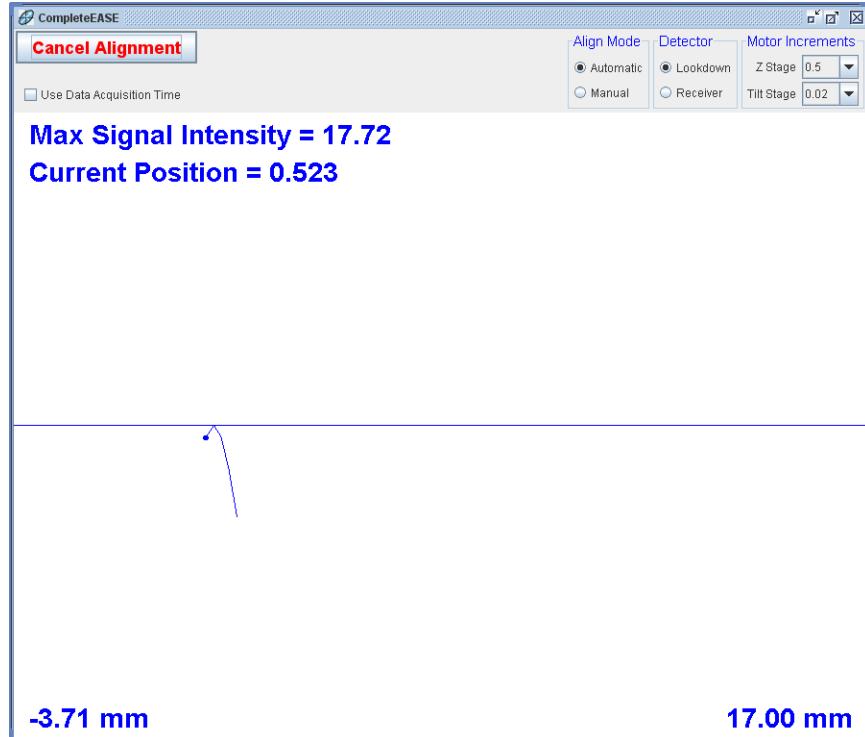


Figure 2-19. Sample Height-Alignment window.

## Common Acquisition Parameters

When finished setting the Acquisition Parameters, you will be asked to save these details in a file. If you will use the same Acquisition Parameters for future measurements, the files can be moved to the Common Folder. Then, they will appear in the drop-down list when selecting your Recipe components. To move Acquisition Parameters into the Common Folder, select the ‘Edit/Create’ Acquisition Parameters button from the Recipe Components box. Next, press the ‘Load’ button from the Acquisition Parameters box, as shown in Figure 2-10. This will open the File Dialog box, as shown in Figure 2-20. Find the Acquisition Parameter Files from the appropriate Folder and then drag them with the mouse from the list of **Files:** in the right to the **Common Folder Links:** location in the left.

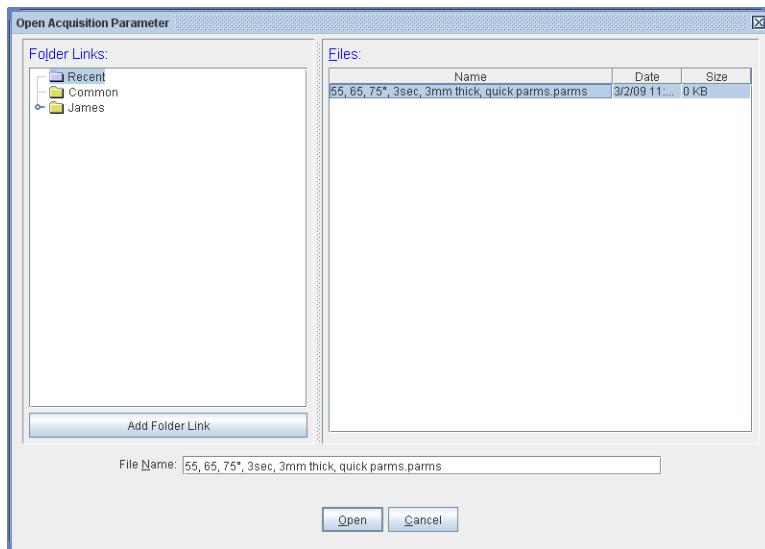


Figure 2-20. When opening Acquisition Parameters, you can find files that you would like to see immediately from the Recipe drop-down menu and drag them into the COMMON folder shown on the left of this box.

## 2.4. Scan Pattern

The Scan Pattern is used to describe where each measurement should be performed across a sample. This option is only needed for ellipsometers with automated sample translation. To make a new Scan Pattern, press ‘Edit/Create’ button to the right of the Scan Pattern selection of the Recipe Components box, as shown in Figure 2-21.

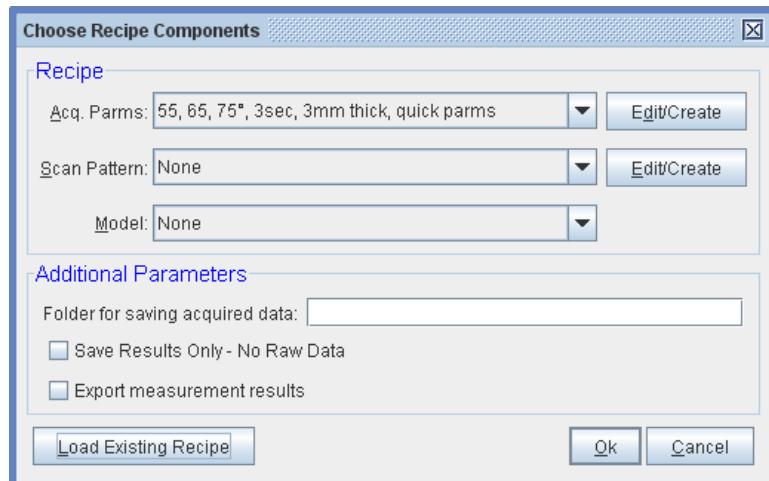


Figure 2-21. Choose ‘Edit/Create’ Scan Pattern from the Recipe Components dialog box.

The Scan Patter Editor, shown in Figure 2-22, allows you to describe both Circular and Rectangular samples. There are many options to automatically fill-in the points to measure, including Grid Fill, R-T Grid Fill, and Line Fill. Most of these selections are intuitive and best learned by testing each button a few times.

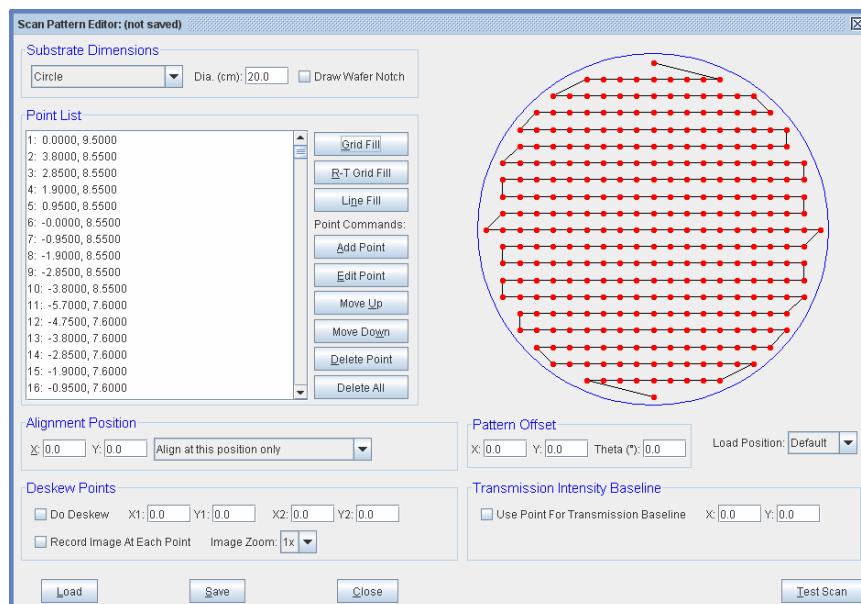


Figure 2-22. Scan Pattern Editor

As an example, if you press the ‘Grid Fill’ button, you will get the options shown in Figure 2-23. The Scan Pattern also describes the overall Alignment methodology. For example, you can choose to Align at a single point only. You can also choose to do a full alignment at the first point and then z-alignment at all other points.

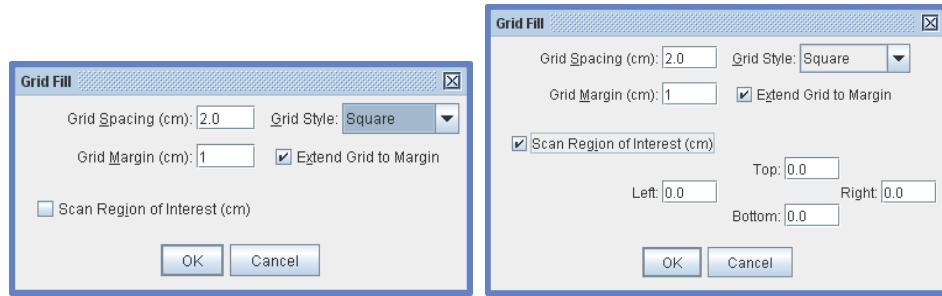


Figure 2-23. Some Grid Fill Options.

## Adding COMMON Scan Patterns

After you have developed Scan Patterns that meet your measurement requirements, you can save these files for future use. If they will be routine patterns, you can add the Scan Patterns to the Common Folder. To accomplish this, press ‘Load’ from the Scan Pattern Editor, as shown in Figure 2-22. This will open the “Open Scan Pattern” dialog box, as shown in Figure 2-24. Find the files you will routinely use and then simply drag them with your mouse from the listing on right to the COMMON folder shown on the left.

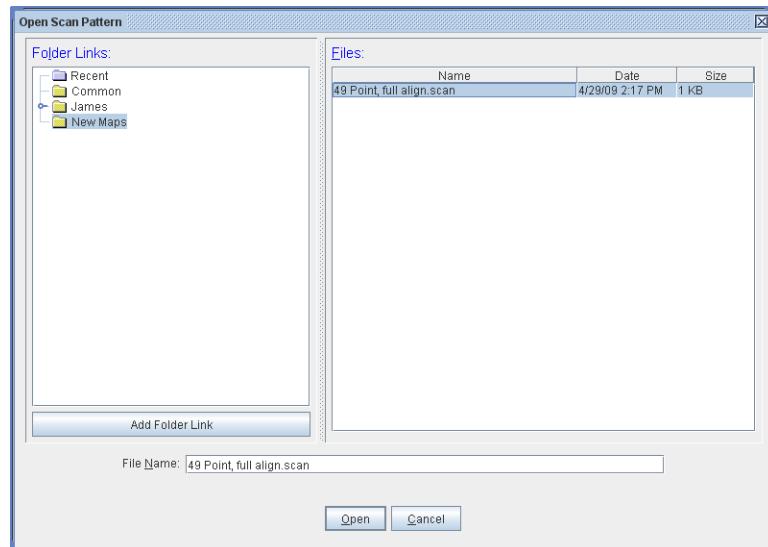


Figure 2-24. Open Scan Pattern Editor. To move routine Scan Pattern files from any location, simply drag them with the mouse from the list on right to the COMMON folder listed to the left of this screen.

## 2.5. Model

A model is a description of how the data will be “fit” by CompleteEASE to determine film thickness and optical constants (or other material properties). Models will be described in significant detail in the upcoming chapters, with examples of how to work with many common models. You can select any model of interest to analyze the data during the recipe. For scans of multiple points, the model will be used to analyze data from each point.

### Common Models

For convenience, you can move Models that are commonly encountered into the “Common” folder. To move into the Common folder location, go to the **Analysis** tab and press ‘Open’ from the **Model:** section. Search for the model of interest and then drag the model name (right side of Figure 2-25) with mouse to the Common folder (left of Figure 2-25). You can do this with multiple models.

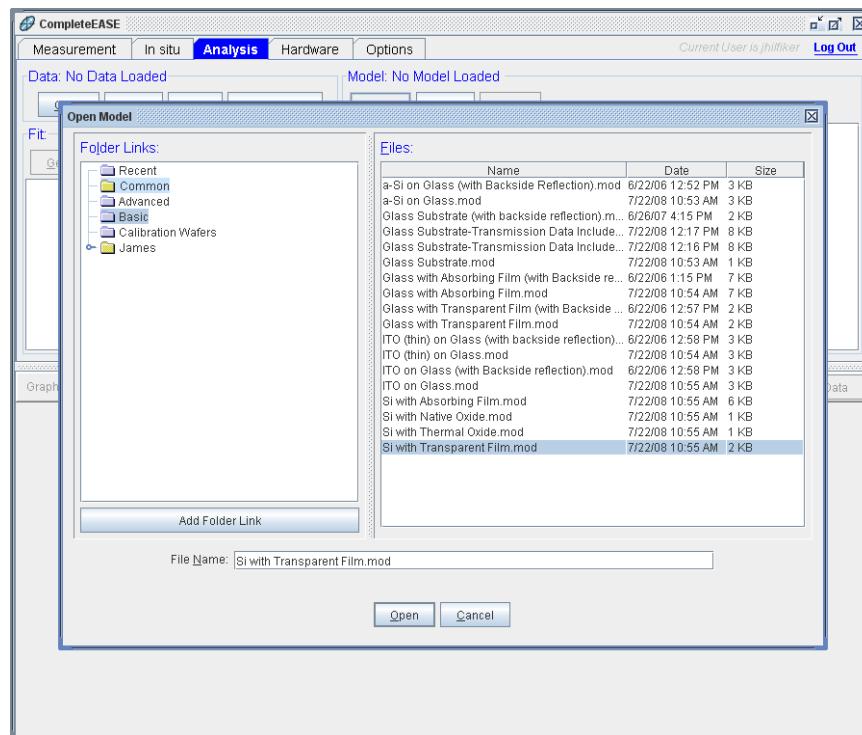


Figure 2-25. From the **Analysis** tab, press ‘Open Model’ and then you can drag-and-drop models from any folder (listed on right) into the Common folder (shown on left).

All models that you move to the Common folder will now appear in the drop-down menu from the Recipe Components box.

## 2.6. Running a Recipe and Viewing Results

After choosing the components of a Recipe, press the ‘Measure’ button. CompleteEASE will collect data per the Acquisition Parameters at each of the locations described in the Scan. After each measurement, the data will be analyzed using the selected Model. An example of this process is shown in Figure 2-26. The **System Status** will show the current hardware operation. The **Fit Results** will be updated with the model fit results from each point. The **Scan Map** will show the current status of a pattern map – green points are already measured, blue is currently being measured, and red are yet to be measured. Finally, the Graph will show the data being collected from the most recent point.

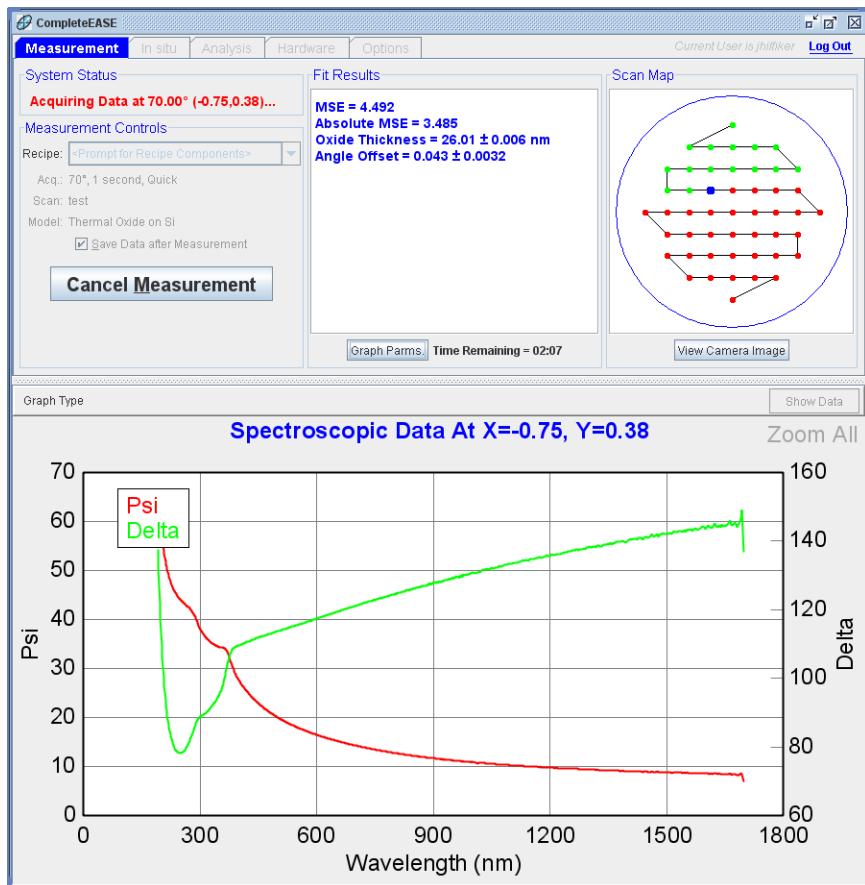


Figure 2-26. CompleteEASE during a Recipe measurement with multiple points.

For maps of multiple points, the Graph can be toggled to Graph the parameters for all points measured up to the current point. To do this, press the ‘Graph Parm’ button within the **Fit Results** section. The parameter to graph can be selected from a drop-down list above the Graph, as shown in Figure 2-27.

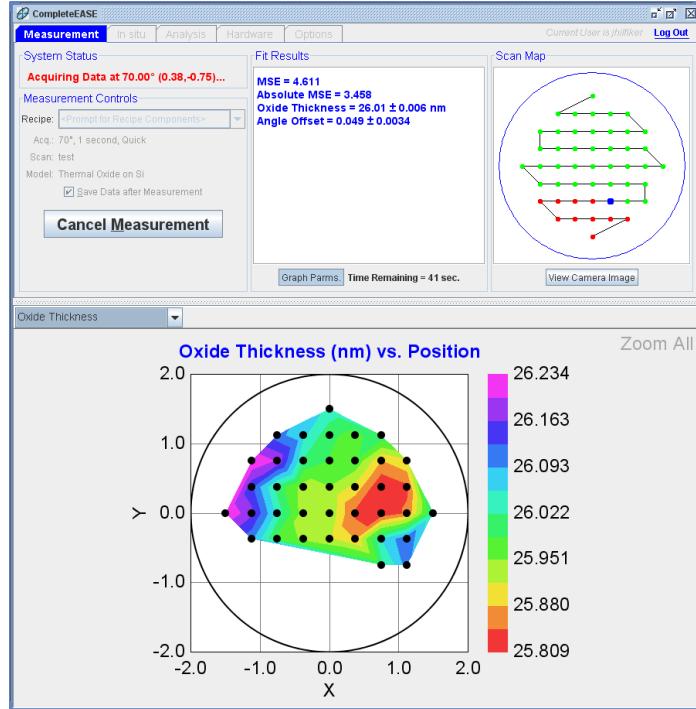


Figure 2-27. Viewing Parameter Results of Scan during Measurement.

When the Scan is completed, a table of results will be presented in the Fit Results panel, as shown in Figure 2-28. The results of any model that are run during recipe are saved with the measurement data and can be opened at a later time by pressing the ‘View Previous Results’ button from the **Fit Results** pane. This opens the window shown in Figure 2-29.

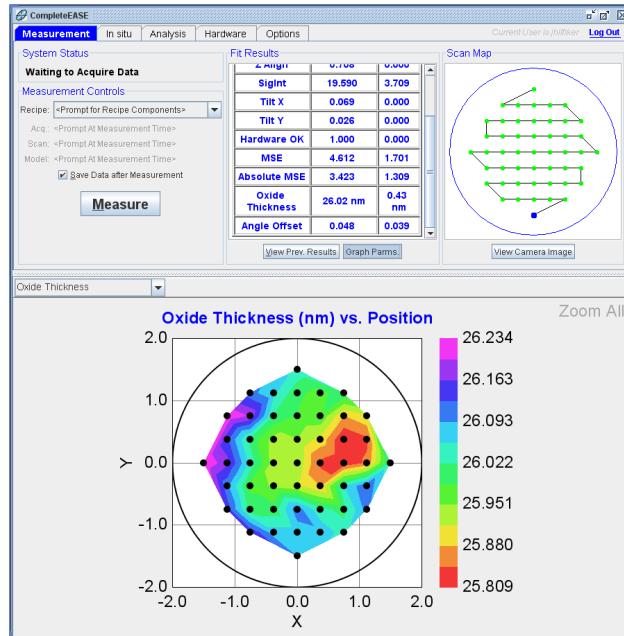


Figure 2-28. Final Results after Scan.

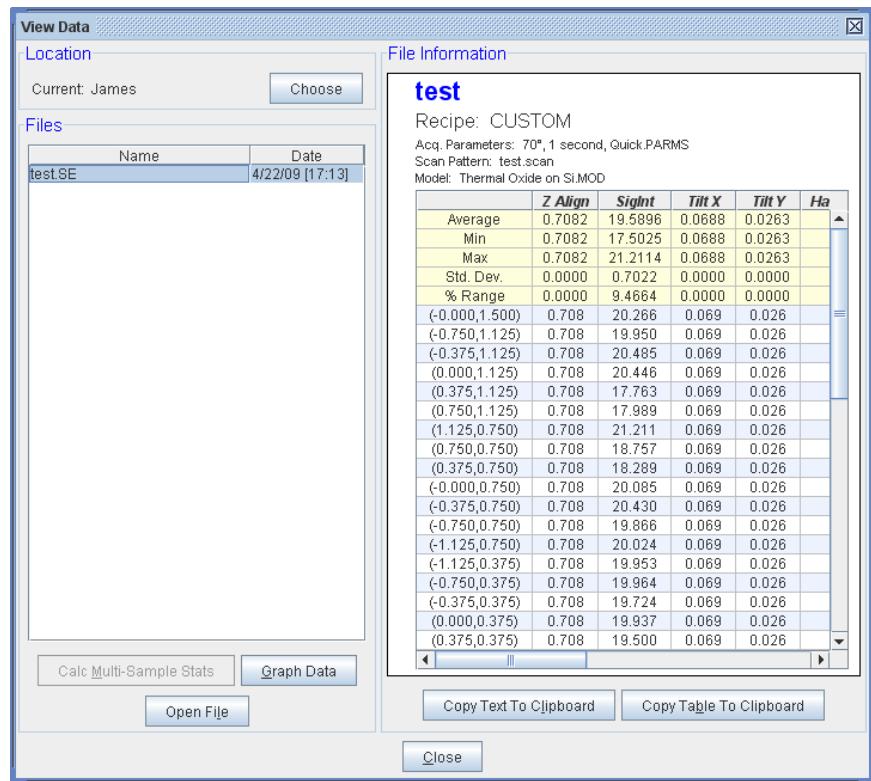


Figure 2-29. Viewing Results after measurements are completed.

# 3. Data Analysis 1 – Basic

We have found that the best way to learn software features is through a series of real-world examples, where the user can follow along. To this end, we have developed examples that spread over multiple chapters to teach the common CompleteEASE data analysis procedures. Following this tutorial is instructive for both beginning and expert users. Chapter 3 begins with basic data analysis examples. Here, we concentrate on thin films that are transparent. Chapter 4 continues with intermediate concepts, concentrating on absorbing materials and the extra difficulties involved with their characterization. Finally, Chapter 5 introduces a few advanced topics.

The section examples from this chapter are listed below, along with the primary CompleteEASE features that are discussed.

## Section 3.1 General Data Analysis Theory

## Section 3.2 Samples with Known N,K: SiO<sub>2</sub> on Si

### FEATURES IN THIS EXAMPLE

- |   |                                     |
|---|-------------------------------------|
| • Opening model and data files                      | • Fitting data                      |
| • Parameter error bars                              | • Hiding or renaming fit parameters |
| • Reporting “derived” parameters                    | • Thickness “Pre-Fitting”           |
| • Defining fit parameters (i.e. turning on and off) |                                     |
| • Visualizing model changes                         |                                     |

## Section 3.3 Transparent Thin Films - 1

### FEATURES IN THIS EXAMPLE

- |                              |                                |
|------------------------------|--------------------------------|
| • Cauchy dispersion equation | • Displaying optical constants |
| • Global fits                | • Expanding layers             |

## Section 3.4 Transparent Substrates

### NEW FEATURES IN THIS EXAMPLE

- |                                  |                               |
|----------------------------------|-------------------------------|
| • Graphing multiple data sets    | • Using the Graph Scratch Pad |
| • Including backside reflections | • Depolarization data         |

### Section 3.5 Transparent Films - 2

| FEATURES IN THIS EXAMPLE      |               |
|-------------------------------|---------------|
| • Surface roughness           | • Grade Layer |
| <b>• Try Alternate Models</b> |               |

### Section 3.6 Log and Report a Series of Films

| FEATURES IN THIS EXAMPLE |  |
|--------------------------|--|
| • Copying to clipboard   | • Comparing optical constants in fit log |
| • HTML clipboard         | • Creating a report                      |
| • Fit log                | • Re-analyzing data from log             |
| • Open/Save Snapshot     |  |

### 3.1. General Data Analysis Theory

Data analysis is a very important part of spectroscopic ellipsometry (SE): without data analysis, SE measures only the ellipsometric parameters Psi and Delta versus wavelength. To determine sample properties of interest, such as layer thicknesses and optical constants, a model-based analysis of the SE data must typically be performed. The only exception to this is in characterizing the optical constants of bulk samples, which is described on the next page. The model-based analysis approach is summarized by the flowchart shown in Figure 3-1. The basic steps of this approach are:

1. SE data is measured on the sample.
2. A layered optical model is built which represents the nominal structure of the sample. This model is used to “generate” SE data.
3. Model fit parameters are defined, and then automatically adjusted by the software to improve the agreement between the measured and model-generated SE data. This is known as “fitting” the data.
4. The results of the fit are evaluated. If the results are not acceptable, the optical model and/or defined fit parameters are modified and the data is fit again.

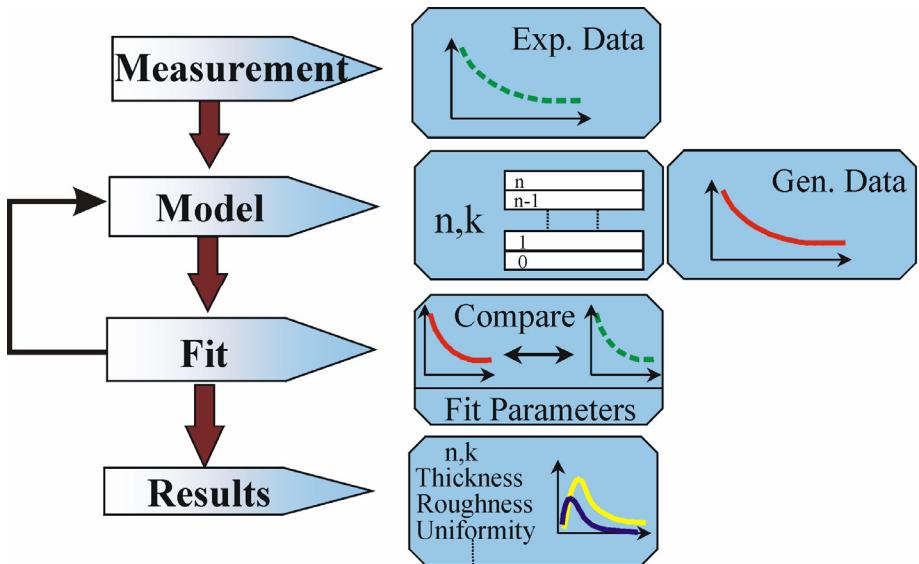


Figure 3-1. SE Data Analysis flowchart.

The above steps will be described in more detail in subsequent sections. Keep in mind that while the basic SE data analysis approach is straightforward, “real-world” samples can often be difficult to analyze. The CompleteEASE software is designed to simplify common SE data analysis procedures which work for many types of samples, but there is no substitute for experience when dealing with complex samples. Please contact your J.A. Woollam Co., Inc. representative if you require assistance.

## “Pseudo” Optical Constants

If SE data is acquired on a bulk sample which does not have any oxide, surface roughness, or any other films or overlayers, then it is possible to directly determine the optical constants of the sample from the ellipsometric data. Equation 4-1 can be used to transform the ellipsometric parameters Psi and Delta into the material optical constants “n” and “k” (or equivalently, the complex dielectric function values “ $\epsilon_1$ ” and “ $\epsilon_2$ ”).

$$\langle \epsilon \rangle = \langle \epsilon_1 \rangle + i\langle \epsilon_2 \rangle = \langle \tilde{n} \rangle^2 = (\langle n \rangle + i\langle k \rangle)^2 = \sin(\phi)^2 \cdot \left[ 1 + \tan(\phi)^2 \cdot \left( \frac{1-\rho}{1+\rho} \right)^2 \right] \quad (2-1)$$

where  $\phi$  is the angle of incidence and  $\rho$  is defined in Equation 1-1.

However, the direct transformation from ellipsometric data to intrinsic material optical properties given by (4-1) is quantitatively valid only if all the assumptions are met, that is, the sample does not have any oxide, surface roughness, or other films or overlayers. Since all these assumptions are rarely met (or at least it is very difficult to independently verify that they are met), the term “pseudo” optical constants is used to describe optical constants which are derived from this analytic transformation. The “ $\langle \rangle$ ” brackets are used to denote “pseudo” optical constants.

In CompleteEASE, pseudo optical constants  $\langle n \rangle$  &  $\langle k \rangle$  (or the pseudo dielectric function  $\langle \epsilon_1 \rangle$  &  $\langle \epsilon_2 \rangle$ ) of the current SE data set can be displayed by selecting the corresponding entry in the “Graph Type:” field of the **Options** tab. Viewing the data in terms of pseudo optical constants can be useful for bulk samples.

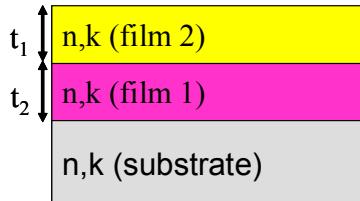
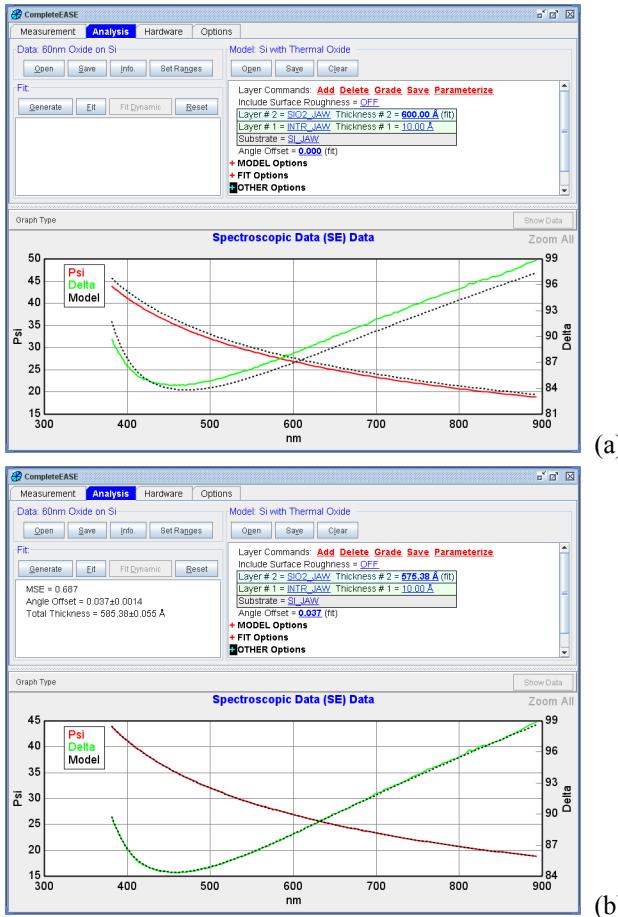


Figure 3-2. Schematic representation of a layered optical model with 2 films, parameterized by thicknesses  $t_1$  and  $t_2$ , and optical constants  $n$  &  $k$ .

## Layered Optical Model

The SE data analysis process for most samples begins by building a layered optical model which corresponds to the nominal sample structure as shown in Figure 3-2. Each layer is parameterized by a thickness ( $t_1$ ,  $t_2$ , etc.) and optical constants. Optical constants describe how light interacts with and propagates through the layer. Using the optical model and standard textbook thin film equations (Snell’s law, Fresnel equations, etc.), the software can calculate “generated” or “simulated” SE data. If the model is a good representation of the sample, the model-generated SE data will be in good agreement with the SE data measured on the sample, as is illustrated in Figure 3-3.



*Figure 3-3. Layered optical model in CompleteEASE, with model generated data: (a) the model generated data (black dashed lines) are not in agreement with the measured SE data (colored curves), (b) when the top layer thickness is adjusted appropriately, the model generated data lies directly on the measured data.*

Sometimes an ideal layered model does not adequately describe the optical behavior of the actual sample. The CompleteEASE software can also model two common “non-idealities”: surface roughness and index gradients. Surface roughness is shown in Figure 3-4: to model the actual sample which may have a non-abrupt “rough” surface, an “effective” roughness layer is added to the model. The optical constants of the “effective” roughness layer are derived by mixing the optical constants of the underlying material with the optical constants of “void” (which has optical constants of  $n=1$ ,  $k=0$ ). The Bruggeman Effective Medium Approximation (EMA) is used to calculate the optical constants of this “mixed” layer assuming 50% void content. While the effective roughness layer approach is certainly an approximation to the actual sample, this approach works extremely well for modeling SE data when the size of the surface roughness is much less than the wavelength of light used to measure the sample. For most SE systems, this implies that surface roughness features must be less than ~40nm.

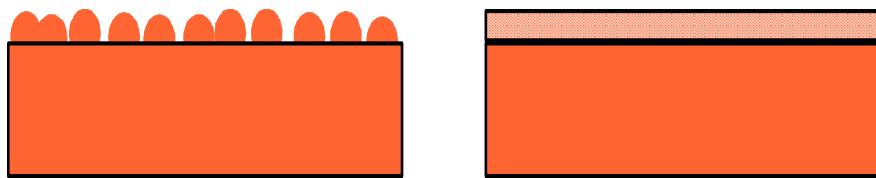


Figure 3-4. Optical model for surface roughness: (a) actual sample with non-abrupt “rough” surface, (b) optical model with “effective” roughness layer.

Sometimes the optical “constants” of a layer are not constant throughout the layer. This may be caused by process variations during the film deposition. Figure 3-5 shows how CompleteEASE can model a “graded” film: the layer is divided into sub-layers with small thicknesses, and each sub-layer has slightly different optical properties. In CompleteEASE, a linear variation in the film index “n” is assumed for the graded layer. This simplified approach, which is automated in CompleteEASE, works well for modeling many types of samples.

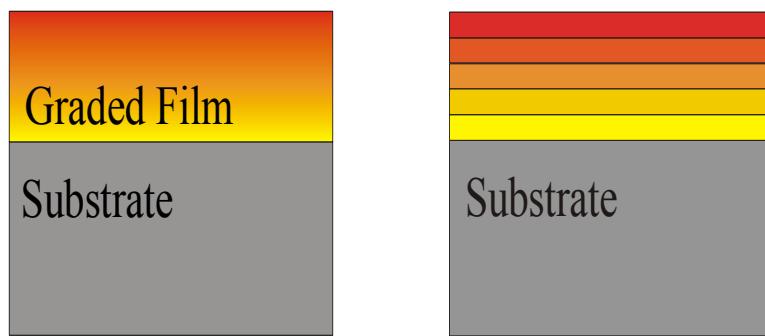


Figure 3-5. (a) Continuous variation in the optical properties of the “graded” film, (b) CompleteEASE approximation of the graded film with discrete layers.

## “Goodness” of Fit: definition of the MSE

Quantifying how well the data generated by the optical model “fits” or “agrees with” the measured data is an important part of the SE data analysis process. One can easily see “by eye” that model (b) in Figure 3-3 fits the data much better than model (a). However, to automate the analysis process, the data fit or “agreement” is quantified by the “MSE” value defined in Eqn. (2-2):

$$MSE = \sqrt{\frac{1}{3n-m} \sum_{i=1}^n [(N_{E_i} - N_{G_i})^2 + (C_{E_i} - C_{G_i})^2 + (S_{E_i} - S_{G_i})^2]} \times 1000 \quad (2-2)$$

where “n” is the number of wavelengths, “m” is the number of fit parameters, and  $N=\text{Cos}(2\Psi)$ ,  $C=\text{Sin}(2\Psi)\text{Cos}(\Delta)$ ,  $S=\text{Sin}(2\Psi)\text{Sin}(\Delta)$

“MSE” is an acronym for Mean Squared Error. Actually, the definition given in (2-2) should be called the “Root Mean Squared Error” (as the error summation is divided by the number of measurement points minus the number of fit parameters, and the square root is taken). However, for historical reasons, we still use the term “MSE” to quantify the “goodness of fit”.

Basically, the MSE sums over all the measurement wavelengths the differences between the measured data (parameters subscripted with “E”) and model generated

data (parameters subscripted with “G”). In CompleteEASE, the difference between the measured and model generated data is calculated in terms of the “N”, “C”, and “S” parameters, which are derived from the ellipsometric Psi ( $\Psi$ ) and Delta ( $\Delta$ ) parameters. The “N, C, & S” parameters have the following properties which make them better suited for the MSE definition (compared to using  $\Psi$  and  $\Delta$ ):

1. N, C, & S are always bounded between -1.0 and 1.0.
2. The rotating compensator ellipsometer configuration measures data with approximately the same precision and accuracy in N, C, & S on any sample.

The N, C, & S parameters for the current data set in CompleteEASE can be plotted by selecting the “N, C, & S” entry in the “Graph Type.” field on the **Options** tab.

The lower the MSE value, the better the fit or “agreement” between the measured and model generated SE data. As the typical precision and accuracy of the measured ellipsometric data in terms of N, C, & S is  $\sim 0.001$ , a multiplicative factor of “1000” is included in the MSE definition of (4-2). This implies that an ideal model fit should have an MSE of  $\sim 1$ . While this is achieved on certain types of samples (single thin films on Si substrates, for example), the best model fits for more complex samples (with thick and/or multiple layers) may exhibit much larger MSE’s ( $> 10$ ) and still be considered acceptable. It is also possible to get an MSE smaller than 1, but this implies the match to data is better than accounted for with random measurement error. In other words, the results likely include some of the “noise” present from data set.

## “Fitting” the Data

To obtain the best fit between the model generated and experimentally measured data (or in other words, to achieve the lowest MSE), parameters of the optical model must be “adjusted”. The user defines which model parameters should be “adjusted” in the fit. These adjustable parameters are also called fit parameters, and they typically consist of layer thicknesses and parameters which define the optical properties of the layers. The CompleteEASE software then uses a standard, iterative, non-linear regression algorithm (the Levenberg-Marquardt method) to automatically minimize the MSE by adjusting the fit parameters. The Levenberg-Marquardt method does an excellent job of quickly converging to the best (lowest) MSE value, assuming that: 1) the optical model accurately represents the sample, and 2) the initial starting values for the fit parameters are reasonably close to their correct (best fit) values. To help ensure that the best fit model is found, the CompleteEASE software includes a couple of powerful features. These features will be used in the data analysis examples which are presented later in this chapter.

- The “Try Alternate Models” command automatically fits the data using the ideal layered optical model, and then with surface roughness and index grading non-idealities added to the model. The results of the various model fits are summarized in tabulated and graphical format, and the user can then decide which model is most appropriate for the sample.
- The “Thickness Pre-Fit” and “Global Fit” options perform a large number of trial fits to the data set, using a wide range of initial starting values for selected fit parameters. The best fit model is then reported.

## Evaluating the Fit Results

Evaluating the fit results is arguably the most important (and unfortunately the most overlooked) aspect of SE data analysis. For a model fit to be acceptable, the following requirements must be simultaneously met:

**1. The model generated data must fit the measured data.**

Unfortunately, this is difficult to quantify exactly, but as a rough guideline the MSE value should be in the 0.5 – 2 range for thin film samples which exhibit relatively little structure in the SE data vs. wavelength curves. For thick film samples with much structure/oscillations in the data, MSE values as high as 10 – 20 may be considered acceptable. Another definition of an “acceptable” fit is that the model generated data lies essentially on top of the measured data set, reproducing all the structures and features (except noise). However, it is not always possible to achieve a perfect fit and still satisfy requirements #2 and #3 below.

**2. The model should be unique.**

The general rule of thumb is to choose the simplest model that adequately fits the data set. It is always possible to reduce the MSE by adding more layers and/or fit parameters to the model, but unless the MSE is significantly reduced, the additional model complexity is not justified. It is not generally possible to guarantee that a given model is unique (i.e., it is the only optical model that can fit the data to the same MSE value). For more complex samples, one should try alternate models and different starting values for the fit parameters to partially verify model uniqueness.

**3. The model and fit parameters must be physical.**

Evaluating this requirement depends on a fundamental understanding of the constituent materials and structure of the sample. For example, if the optical constants determined from a model fit are outside acceptable bounds for the material (e.g.,  $k < 0$  or  $n > 10$ ), the results are unphysical and should be considered invalid. Often, a knowledge base of measurements on similar samples is helpful in evaluating the “believability” of the fit results. For example, from experience we know that index gradients would be acceptable (or even expected) when analyzing data acquired on indium tin oxide (ITO) films, but a model which reported an index gradient when analyzing a thermal oxide on silicon sample would be questionable. Complementary techniques such as stylus profilometry, AFM, XTEM, SIMS or Auger depth profiling can also be used to corroborate the physicality of the model fit results.

If the model fit is deemed unacceptable, try modifying the optical model and/or defined fit parameters, and repeat the fit procedure until an acceptable fit is achieved. Finding an acceptable balance between the quality of the fit and the model complexity requires patience and experience.

## “Physical” Optical Constants

One important criterion for any model is that the resulting optical constants do not have an “unphysical” shape. This can be difficult to evaluate without experience. To help “jump-start” your understanding of optical constants, we show a few examples of material optical constants and explain what makes their shape “physical”. We will also show corresponding results that would be “unphysical”.

- A. Index (n) must increase toward shorter wavelengths when the material is transparent ( $k=0$ ).**

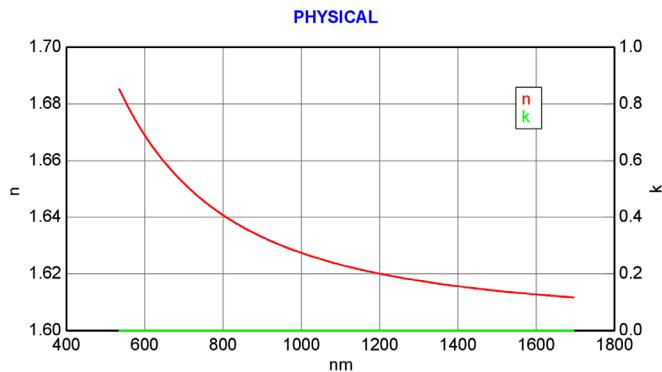


Figure 3-6. Index must increase toward shorter wavelengths if  $k=0$ . These optical constants are physical as they obey this rule.

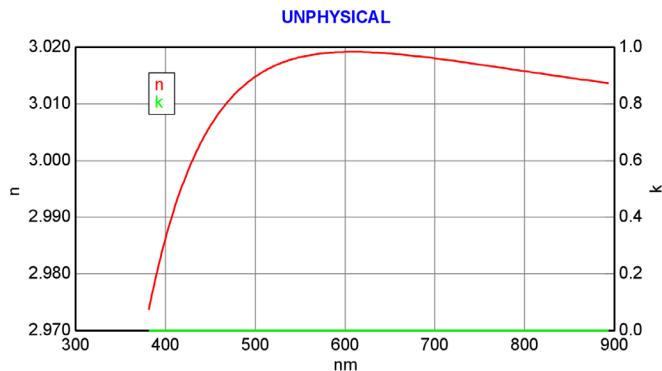


Figure 3-7. Index must increase toward shorter wavelengths if  $k=0$ . These optical constants are not physical because  $n$  turns-over (decreasing toward shorter wavelengths) below 600nm without any absorption ( $k=0$ ).

- B. Index (n) will “turn-over” and decrease toward shorter wavelengths if material becomes absorbing ( $k$  increasing).**

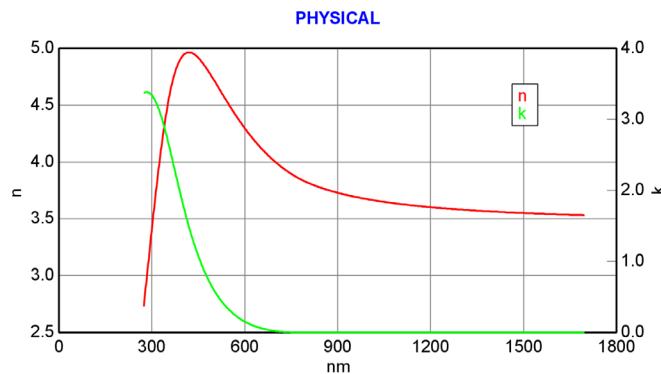


Figure 3-8. Index will turn-over and decrease toward shorter wavelengths when material becomes absorbing ( $k$  increasing toward shorter wavelengths). These optical constants are physical as they obey this rule.

- C. Index (n) will return to the normal behavior of increasing toward shorter wavelengths as the amount of absorption begins to decrease ( $k$  decreasing).**

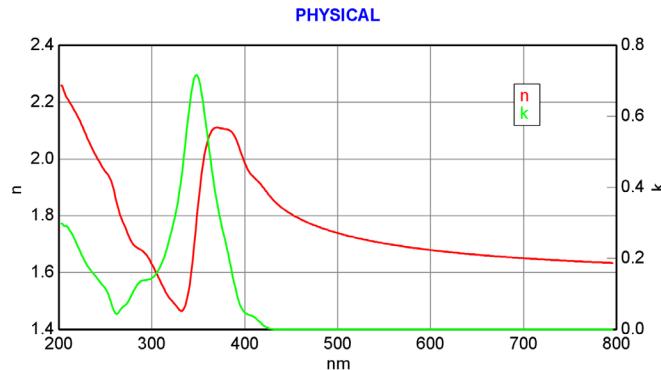


Figure 3-9. Graphed optical constants appear “physical”, as the index is increasing for wavelengths above 400nm (where  $k = 0$ ), index turns-over when absorption becomes larger (near 350nm) and then returns to normal shape with increasing toward short wavelengths when the absorption decreases (below 320nm).

- D. Extinction coefficient (k) cannot be negative.**

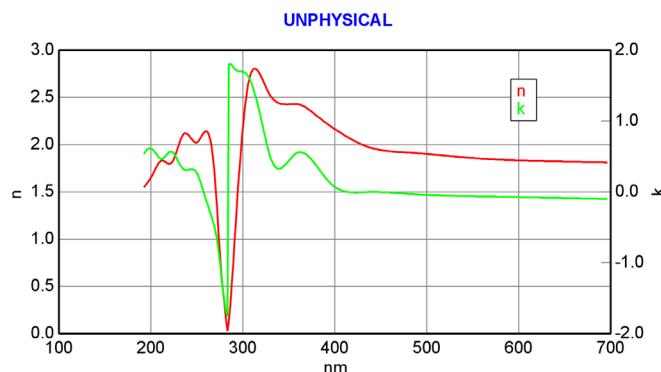


Figure 3-10. The graphed optical constants are “unphysical” because the extinction coefficient,  $k$ , goes negative.

## 3.2. Samples with Known N,K: SiO<sub>2</sub> on Si

| FEATURES IN THIS EXAMPLE                            |                                     |
|---|-------------------------------------|
| • Opening model and data files                      | • Fitting data                      |
| • Parameter error bars                              | • Hiding or renaming fit parameters |
| • Reporting “derived” parameters                    | • Thickness “Pre-Fitting”           |
| • Defining fit parameters (i.e. turning on and off) |                                     |
| • Visualizing model changes                         |                                     |

The simplest types of samples to analyze are those in which the optical constants of each material are known. For this case, only layer thickness needs to be determined in the optical model fit. Unfortunately, most samples do not fall into this category, as the “optical constants” for most materials are rarely constant. Instead, they often depend on the material deposition and processing conditions. The analysis examples in the following sections demonstrate how to determine both layer thickness and optical constants from SE data. However, in this section we show the “classic” ellipsometry example which assumes known optical constants for the materials: thermally-grown silicon dioxide films on silicon wafer substrates (SiO<sub>2</sub> on Si).

For high quality thermally grown oxide films on semiconductor-grade Si wafers, the optical constants of both the Si wafer substrate and the SiO<sub>2</sub> film are known to be constant. The CompleteEASE software has a standard model for analyzing this type of sample. To open this model:

1. Start the CompleteEASE software (if the program is not open).
2. Select **Analysis>Model** >‘Open’.
3. Highlight (by clicking) the “Basic” folder in the “Location” list on the left side of the screen.
4. Select “Si with Thermal Oxide.mod” in the “Files:” section and click ‘Open’ button.

Next, open an example data file that we previously acquired on an ellipsometer system:

1. Select **Analysis>Data** >‘Open’.
2. Highlight the “Examples” folder in the “Location” list .
3. Select the “25nm Oxide on Si.SE” file.
4. Click the ‘Open’ button to open the selected data file.

After opening the specified model and data files, the CompleteEASE screen should appear as shown in Figure 3-11. Note the experimentally measured SE data (the ellipsometric Psi and Delta parameters versus wavelength) appear in the graph panel as red and green curves, and the optical model contains a substrate (SI\_JAW) and two layers (INTR\_JAW and SIO2\_JAW).

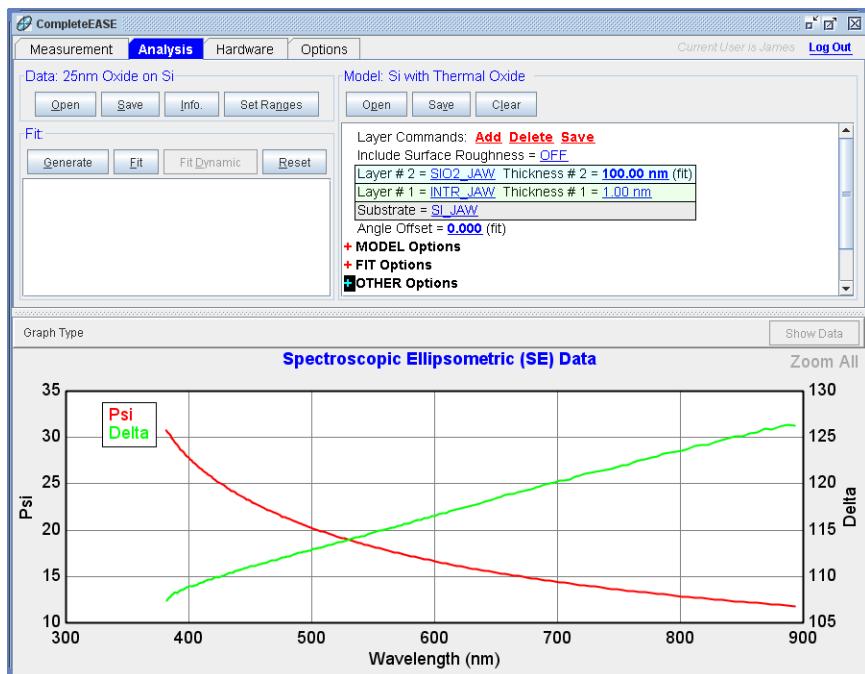


Figure 3-11. CompleteEASE screen after opening the “Oxide on Si” model and the “25nm Oxide on Si” example data.

## Fit Results and Parameter Error Bars

To analyze the data, click on *Analysis*>*Fit*>‘Fit’. The analysis will proceed very quickly (less than one second on most computers) and the fit results will be displayed in the **Fit** section (Figure 3-12). Of course, the main parameter of interest is the total film thickness (27.42nm). The value after the “ $\pm$ ” is the estimated error bar on each fit parameter.

The error bar values reported by CompleteEASE come from the 90% confidence intervals that are calculated by the fit algorithm. Since the confidence interval calculation makes a number of statistical assumptions that are not in general rigorously satisfied, the error bar values reported by CompleteEASE should not be literally interpreted. In practice, the error bars provide an estimation of the measurement reproducibility. Large error bars (relative to the magnitude of the fit parameter) are a useful indicator that the model is not sensitive to the parameter (and the parameter should likely be removed from the fit). The “Total Thickness” parameter is a derived parameter (more on that later). Its error bar is calculated from the sum of error bars for each varied thickness in the fit. Also note that after the fit, the black dashed “Model” generated data curves are essentially on top of the colored experimental data curves.

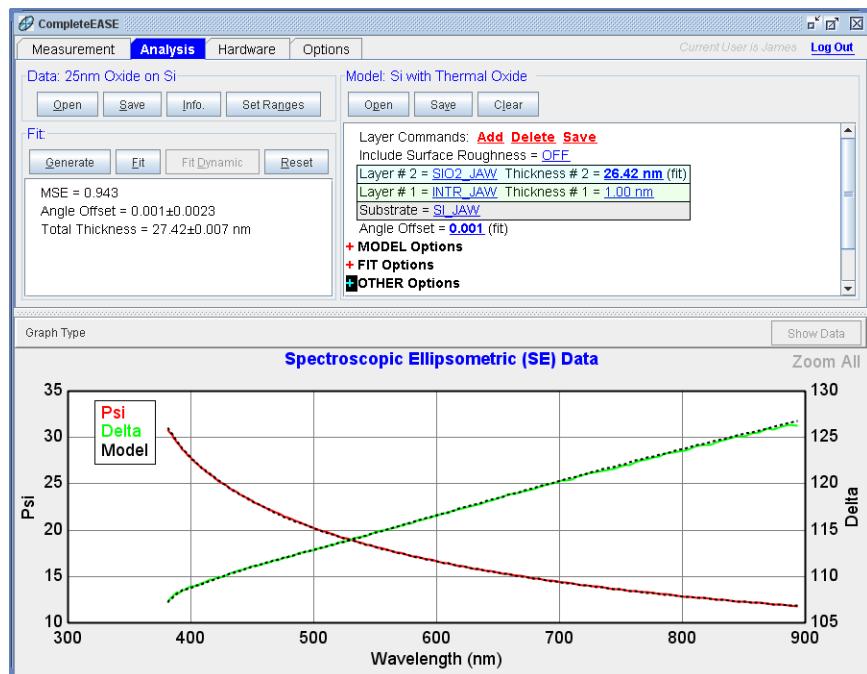


Figure 3-12. SE data fit and results for oxide on Si sample.

As an exercise, use the “Si with Thermal Oxide” model to determine the total film thickness for each oxide on Si example file: “60nm Oxide on Si”, “120nm Oxide on Si”, “300nm Oxide on Si”, and “1600nm Oxide on Si”. Open each data file (**Analysis>Data**)>‘Open’) and click ‘Fit’; the results should agree with the values shown in Table 3-1. There are a few important trends to note in this table:

1. The MSE increases with thicker films (from ~1 to >10), though all data fits are very good to the eye (i.e. black dashed Model curves lie on colored experimental curves).
2. The reported “Total Thickness” values do not agree exactly with thicknesses given in the file names (this is acceptable, as the file names are only estimated film thickness values).

Table 3-1. Fit results from “Oxide on Si” example files.

| Example File       | MSE    | Angle Offset    | Total Thickness (nm) |
|--------------------|--------|-----------------|----------------------|
| 25nm Oxide on Si   | 0.943  | 0.001 ± 0.0023  | 27.42 ± 0.007 nm     |
| 60nm Oxide on Si   | 0.687  | 0.037 ± 0.0014  | 58.54 ± 0.006 nm     |
| 120nm Oxide on Si  | 2.510  | 0.071 ± 0.0044  | 124.61 ± 0.007 nm    |
| 300nm Oxide on Si  | 3.673  | -0.051 ± 0.0070 | 273.02 ± 0.014 nm    |
| 1600nm Oxide on Si | 13.885 | -0.094 ± 0.0261 | 1640.58 ± 0.195 nm   |

## JAW Oxide on Si Model, with Interfacial Layer

The J.A. Woollam Co. “Si with Thermal Oxide” optical model supplied with the CompleteEASE software has a number of unique features. First, the oxide film is modeled as 2 layers: INTR\_JAW, which is a higher-index interface layer, and SIO2\_JAW, which contains the optical constants for the SiO<sub>2</sub> film (which are different from the optical constants of a SiO<sub>2</sub> “fused silica” bulk sample). The optical constants for these layers and for the SI\_JAW substrate were published by Herzinger et al.<sup>1</sup> The interface layer adds model complexity, but it significantly improves the data fit when the model is applied over a wide oxide thickness range.

*Turn fit parameters on/off by right-click of mouse on the parameter value.*

To simplify the model and provide more unique fit results, the interface layer (“Thickness #1”) is fixed at 1nm. This value is typical for thinner oxide films (thickness < 100nm); while for thicker oxides, a slight fit improvement can be obtained by also fitting the interface layer thickness. For example, open the “1600nm Oxide on Si” file and fit the data with the “Si with Thermal Oxide” model. Now add the interface layer thickness as a fit parameter by right-clicking the mouse on the “Thickness #1” value (that is, ( $\text{Ctrl}$ R) on “1 nm”). The value is now shown in a bold font followed by the word “(fit)”, indicating that this value is now defined as a fit parameter. (To turn “off” a fit parameter, simply right-click ( $\text{Ctrl}$ R) again on the parameter value.) Click on the ‘Fit’ button, and the results box shown in Figure 3-13 should appear. Note the fit value for Thickness #1 is 3.48 (an increase from the nominal value of 1nm) and the MSE is reduced slightly from 13.885 to 10.316. Unless the explicit goal of the sample analysis is to characterize the interface thickness, it is best to fix Thickness #1 at 1nm nominal value.

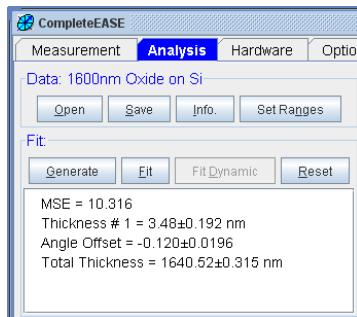


Figure 3-13. Results from “Si with Thermal Oxide” model fit to “1600nm Oxide on Si” data with interface layer (“Thickness #1”) added as a fit parameter.

## Derived Parameters

Even though the interface thickness increased in the preceding fit, the Total Thickness remained essentially the same (1640.58 vs. 1640.52 nm) for both fits. The “Total Thickness” is not an actual fit parameter, as the value is “derived” by summing all layer thicknesses in the model. Derived parameters can be added to the results by turning “ON” the “Include Derived Parameters” option within **Model >+FIT Options** (Figure 3-14). In addition to “Total Thickness”, additional derived parameters include “n” and “k” values for a specified layer and wavelength, optical thickness, total optical thickness and many other possibilities. These will be addressed further in a later example.

<sup>1</sup> C.M. Herzinger, B. Johs, W.A. McGahan, J.A. Woollam, and W. Paulson, “Ellipsometric determination of optical constants for silicon and thermally grown silicon dioxide via a multi-sample, multi-wavelength, multi-angle investigation”, *J. Appl. Phys.* **83** (1998) 3323.

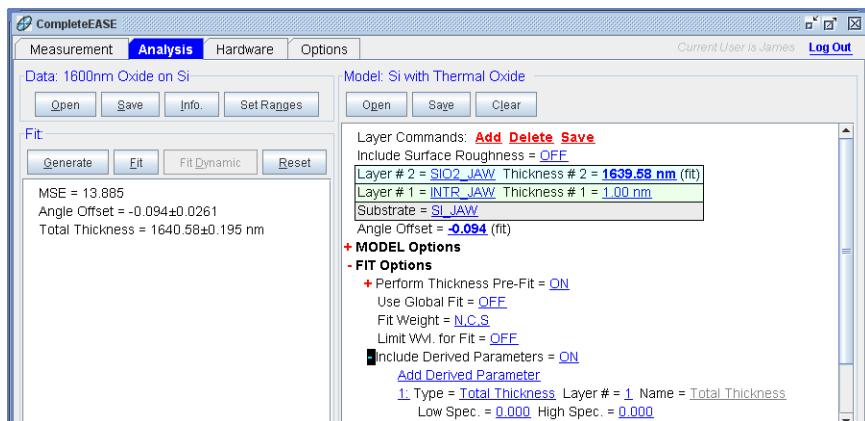


Figure 3-14. “Include Derived Parameter” section of the model.

If you wish to delete a Derived Parameters, simply right-click on the number (shown in blue) next to the parameter you wish to delete.

## Hiding, Renaming, and Bounding Fit Parameters

In the “Si with Thermal Oxide” model, “Angle Offset” was also defined as a fit parameter. The “Angle Offset” is added to the nominal angle of incidence in the optical model calculation. For most analysis (and especially when fitting for optical constants) it is best to leave the Angle Offset fixed at 0. However, since the Si and oxide optical constants are well known and there is only one additional fit parameter in the model (Thickness #2), fitting the “Angle Offset” can slightly improve the SiO<sub>2</sub> thickness analysis results by compensating for small sample alignment errors. Best sensitivity to angle of incidence occurs for thin layers (<100nm).

“Thickness #2” is a fit parameter in the analysis, but this parameter doesn’t show up in the fit results. “Thickness #2” was hidden to prevent confusion with the “Total Thickness” that is reported. To hide a fit parameter so that it is not displayed in the Results, left-click ( $\text{Ctrl}+\text{L}$ ) on the fit parameter value. For example, if you ( $\text{Ctrl}+\text{L}$ ) on “1637.05 nm”, the dialog box shown in Figure 3-15(a) will appear. “Minimum” and “Maximum” values for the parameter can be specified to bound the parameter space for the fit. If the “Show Adv. Parameters” box is checked, the Parameter Name, Error Bars, and Specification sections are visible. If the “Hide” box is checked, the fit parameter value will not be displayed as a fit result.

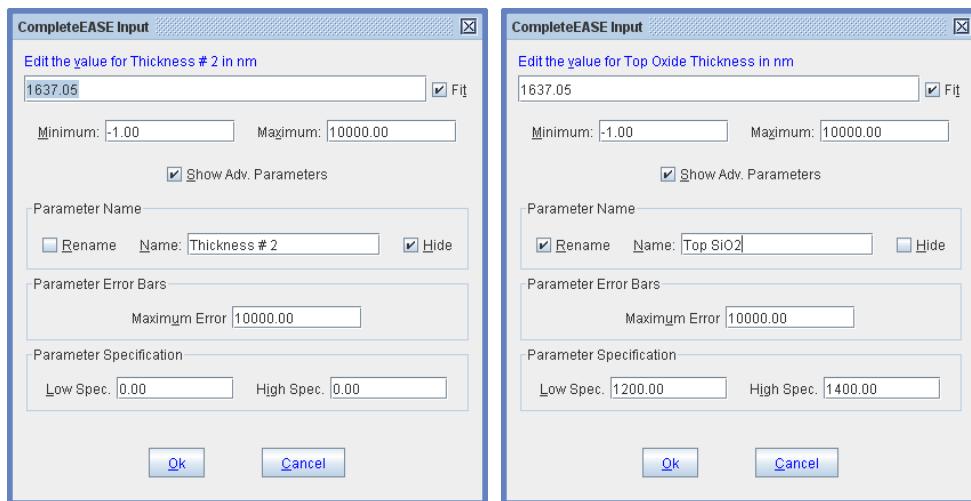


Figure 3-15. Fit parameter dialogs, showing how to (a) “Hide” or (b) “Rename” fit parameters. High and Low specs for the fit parameter are also set in (b).

Edit “Thickness #2” as shown in the Figure 3-15(b) dialog box:

- Check the “Rename” box, type in a different “Name:” for the parameter (e.g., “Top SiO2”)
- Uncheck the “Hide” box
- Type in values for “Low Spec.” (1200) and “High Spec.” (1400).

Click “Ok” to close the dialog box, and fit the data again (with the “1600nm Oxide on Si” data file loaded). Fit results will appear as shown in Figure 3-16. Since the “Top SiO2” value (1639.58) is outside the Low and High parameter Spec (1200 – 1400), an (Out Of Spec.) message appears after the result.

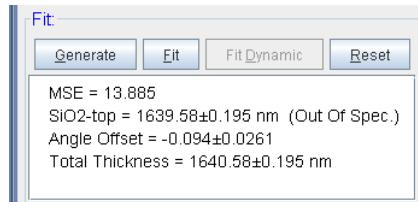


Figure 3-16. Fit results with parameter renamed and “Top SiO2” parameter “Out-of-Spec”.

## Thickness Pre-fitting

One further concept will be demonstrated using “Si with Thermal Oxide” model. For this example, reload both the “Si with Thermal Oxide” model and the “1600nm Oxide on Si” example data file. From the **Model>+FIT Options** section, turn the “Perform Thickness Pre-Fit” option to “OFF” by clicking on the underlined blue value. Then press **Fit>‘Generate’**. The screen should appear as shown in Figure 3-17. Note that the data generated by the model (black dashed curves) using the default thickness (100nm) does not match the experimental data. Now click the ‘Fit’ button: the data fit is still very poor, and the reported MSE is very high (677). This illustrates what happens if you start the fit with parameter values that are not reasonably close to their best fit values.

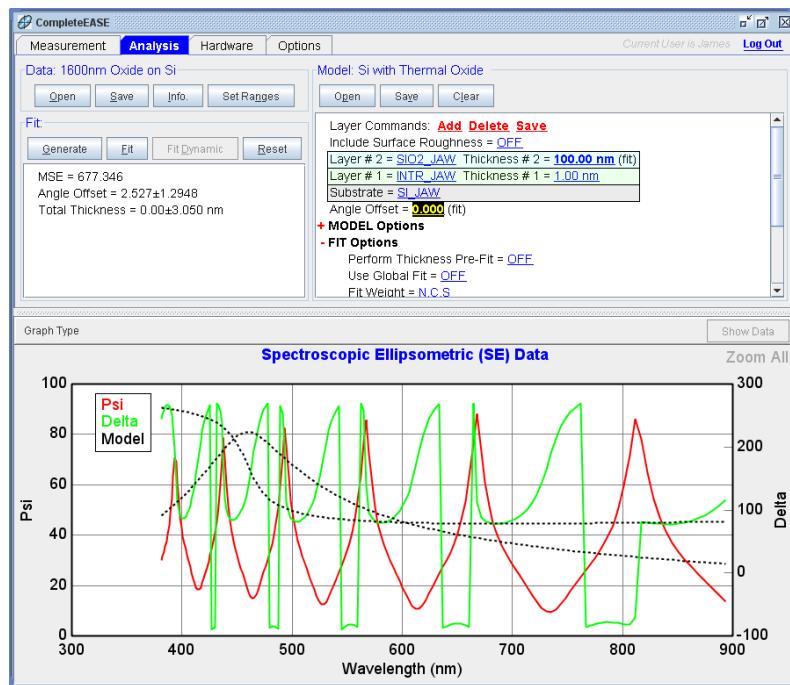


Figure 3-17. Data generated from “Si with Thermal Oxide” model, using default parameter values. The “Perform Thickness Pre-Fit” option is turned “OFF”.

Now set “Thickness #2” to “1650” and “Angle Offset” to “0” (by clicking on the respective parameter values), and click “Generate”. The screen should appear as in Figure 3-18. While the model and experimental data curves do not line up exactly (slight shift), at least the basic structure and features in the data sets appear similar. Click the ‘Fit’ button, and observe that a good quality fit is obtained.

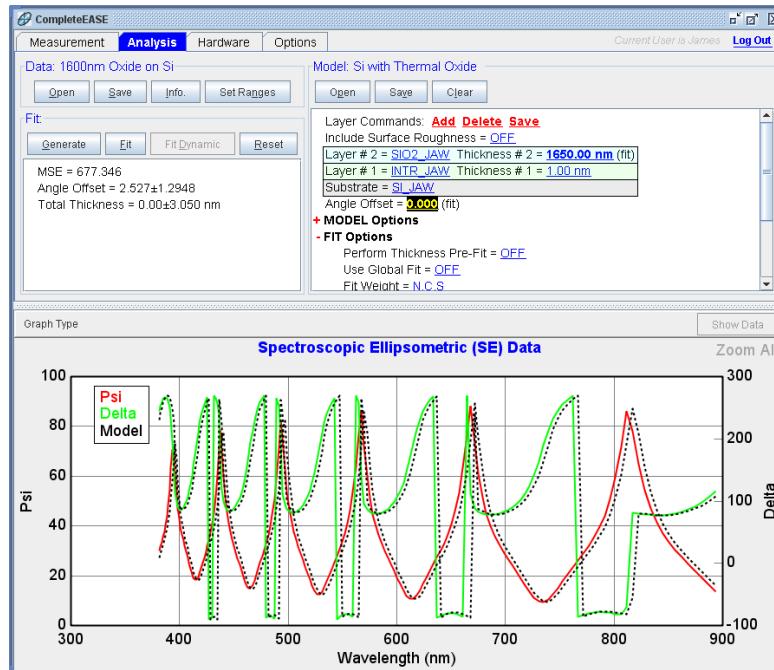
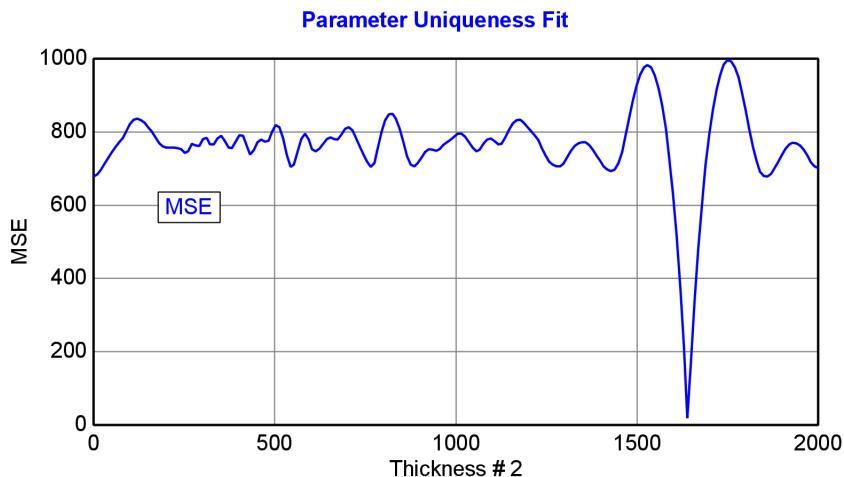


Figure 3-18. “1600nm Oxide on Si” data set, with model data generated using a closer (1600nm) starting thickness value.

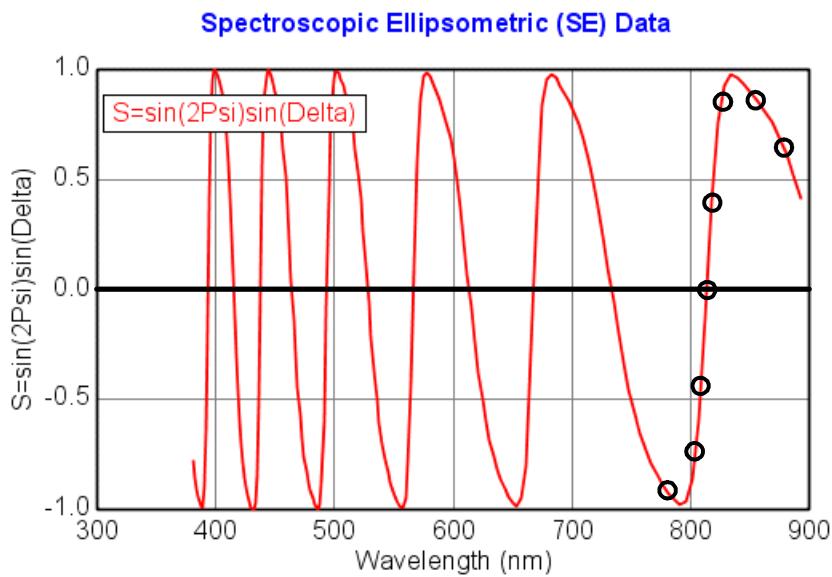
A good starting value for “Thickness #2” is critical to achieve the best data fit. Without the Thickness PreFit, the software tries to adjust the fit parameter (thickness) to lower the MSE. However, the MSE profile is not a single minimum at the correct thickness. It also contains many other minima, which are called local minima. These local minima can trap the normal fit process. Each of these local minima are at a much larger MSE value, as shown in Figure 3-19., so it is easy to distinguish the correct answer from a thickness result that does NOT match the Experimental curves. However, it is tedious to guess starting film thickness values for all samples.



*Figure 3-19. MSE profile for 1600nm SiO<sub>2</sub> on Silicon data using the Thermal Oxide on Silicon model. The only answer occurs when the SiO<sub>2</sub> thickness is near 1640nm. However, a normal fit will only find this answer if the starting point is near the final answer. To overcome this problem, our patented “Thickness PreFit” automatically searches for a good starting thickness near the final answer.*

The CompleteEASE “Thickness Pre-Fit” option automatically provides a good starting value for the thickest layer in the model, using a special patent-pending algorithm. To demonstrate this feature, turn the “Perform Thickness Pre-Fit” option back to “ON”. Input a “bad” starting value for the “Thickness #2” parameter, for example “50”. Click ‘Generate’ to verify that the model starting parameters are not close to the best fit. Now when you click the ‘Fit’ button, a good data fit appears on the screen, even though the initial thickness value (50nm) was not close to the final best fit value (1639.58nm). For most analysis, it is useful to have the “Perform Thickness Pre-Fit” option turned “ON”, especially if accurate starting thickness values are not available.

To better understand the Thickness Prefit, consider that the data will oscillate versus wavelength as the film becomes thicker due to interference between reflected light from the surface and bottom of a thin film. As thickness increases, more oscillations will occur versus wavelength. Of course this is not independent of the index of refraction, but the underlying principle is that a larger “optical thickness” will have more oscillations. The Thickness Prefit works by quickly interpreting the data oscillations to “estimate” the actual thickness, as illustrated in Figure 3-20. Often, this fast calculation is adequate to get a good starting point for the normal fit procedures.



*Figure 3-20. Thickness Prefit uses a proprietary algorithm to very quickly estimate the thickness of a film based on oscillations in the data.*

## Visualizing Model Changes

It is useful to understand how changes in the model affect the generated data. For example, an increase in thickness will shift the interference oscillations toward longer wavelengths. CompleteEASE allows convenient simulation as a model parameter changes.

- Position the mouse over a model parameter you wish to adjust.
- Hold down the “Shift” key as you roll the mouse wheel up and down. The model parameter is increased or decreased by a set increment and data are re-generated with the new model values.
- For smaller parameter increments, simultaneously hold “Ctrl-Shift” as you roll the mouse wheel.

### 3.3. Transparent Thin Films - 1

| FEATURES IN THIS EXAMPLE   |   |
|--|---|
| <ul style="list-style-type: none"><li>• Cauchy dispersion equation</li><li>• Global Fits</li></ul> | <ul style="list-style-type: none"><li>• Displaying optical constants</li><li>• Expanding Layers</li></ul> |

The next set of examples will demonstrate how to determine the film thickness and index of refraction “n” for transparent films deposited on substrates with known optical constants. While there are certainly cases in which it is not known *a priori* if the film is transparent (films which are absorbing are covered in the following chapter), there are also many applications where the film can be assumed transparent, at least in the visible spectral range: optical coating materials ( $\text{SiO}_2$ ,  $\text{TiO}_2$ ,  $\text{Ta}_2\text{O}_5$ ,  $\text{MgF}_2$  etc.), some nitrides ( $\text{Si}_3\text{N}_4$ ,  $\text{AlN}$ ), many organic films (photoresists, PMMA, spin-on polymers, etc.), and so on. In addition, the presence of periodic data oscillations suggests interference between top and bottom of a semi-transparent film (as shown in Figure 3-21).

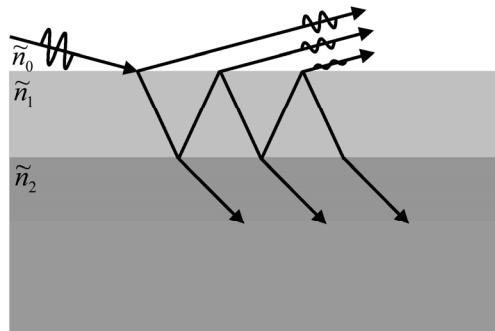


Figure 3-21. Interference within a transparent thin film.

The index of refraction for transparent films in the visible spectral range is often specified using the Cauchy dispersion relation given by Eqn. 4-3. The “An” parameter relates to the approximate amplitude for the material index, while “Bn” and “Cn” parameters provide the shape or curvature of the index versus wavelength. Figure 3-22 shows index dispersion curves for three common transparent materials. For most transparent materials in the visible spectral range, the index curves slightly upward at shorter wavelengths, a behavior which is well described by the Cauchy dispersion equation.

$$n(\lambda) = A_n + \frac{B_n}{\lambda^2} + \frac{C_n}{\lambda^4} \quad (4-3)$$

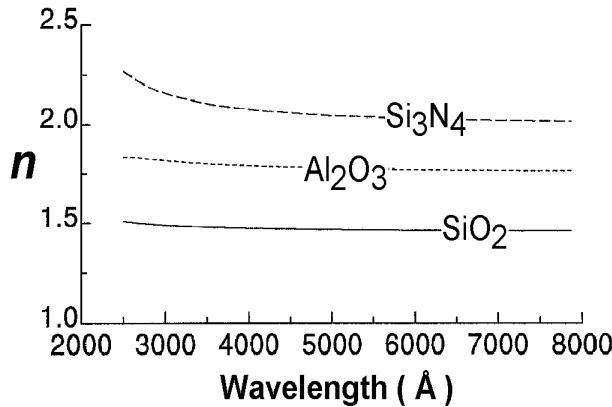


Figure 3-22. Index of refraction “*n*” for common transparent materials, described by the Cauchy dispersion equation.

## Si with Transparent Film

This example uses the “Flow-on Glass on Si” example data file. First, fit this data set using the “Si with Thermal Oxide” model as described in the preceding section. The results should look like Figure 3-23; the data fit is reasonable, but discrepancies are observed between the model and experimental curves in certain spectral regions, and the MSE is fairly high (~28). The “Flow-on Glass” material coated on this sample is similar to  $\text{SiO}_2$ , but with slightly different refractive index.

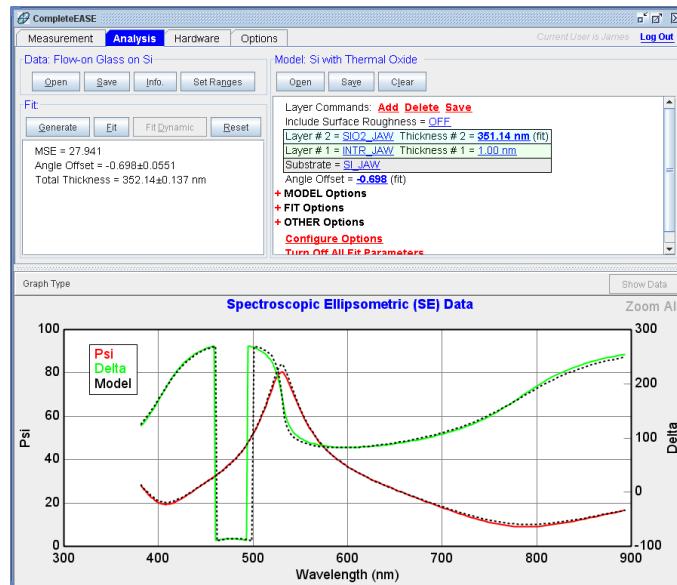


Figure 3-23. Fit using “Si with Thermal Oxide” model.

To determine the index and thickness of the Flow-on Glass film, open the “Si with Transparent Film” model (which is also found under the “Basic” folder in the Open Model dialog box), and click the ‘Fit’ button. A nice data fit is obtained (though the fit takes longer than the “Si with Thermal Oxide” data fit) with the fit results shown in Figure 3-24. The reported fit parameters are Thickness #1 (which is the film thickness) and the film’s Cauchy parameters: A, B, and C. The film index of refraction at a specified wavelength (632.8nm) is also reported as a derived parameter.

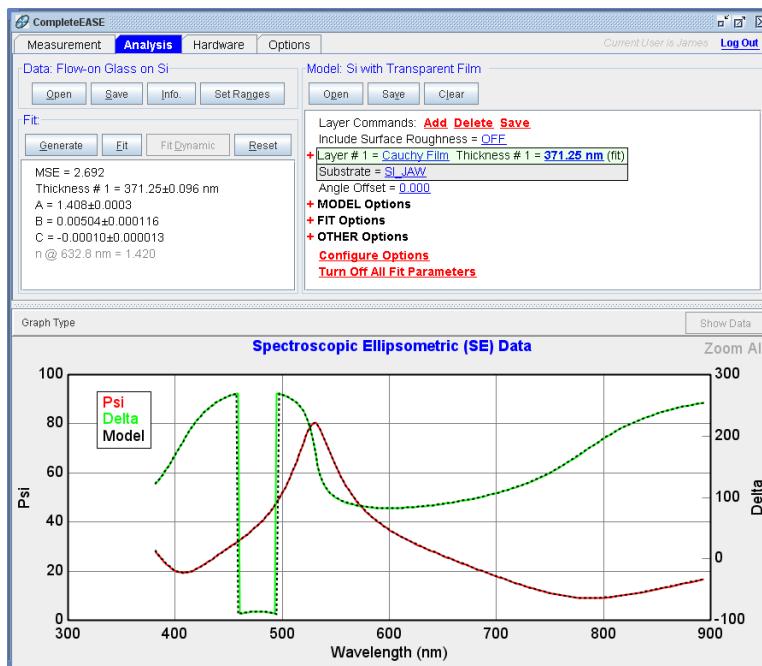


Figure 3-24. Fit results for “Flow-on Glass on Si” example file using the “Si with Transparent Film” model.

*Right-click the mouse ( $\text{Ctrl} + \text{R}$ ) over a Layer name to show its optical constants ( $n, k$ ).*

To display the film’s index of refraction versus wavelength, right-click ( $\text{Ctrl} + \text{R}$ ) on the material name “Cauchy Film” and choose the option “Graph Layer Optical Constants” (Figure 3-25). The optical constants will be displayed in the graph window as shown in Figure 3-26.

To display and edit the film Cauchy parameters, click ( $\text{Ctrl} + \text{L}$ ) the red “+” symbol to the left of “Layer #1”. The layer expands (and the “+” turns to a “-”, which can be clicked to collapse the layer), and the layer fit parameters are now accessible, as shown in Figure 3-26. The “k Amplitude”, “Exponent”, and “Band Edge” parameters describe an exponential “Urbach” absorption tail - not required for this example.

**NOTE:** The Cauchy layer is described in further detail in Section 8.5

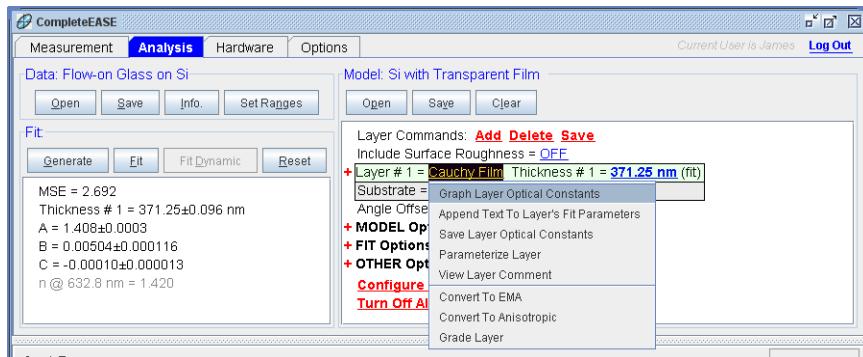


Figure 3-25. To view a layer optical constants, ( $\text{Ctrl} + \text{R}$ ) over the layer name and choose to “Graph Layer Optical Constants”.

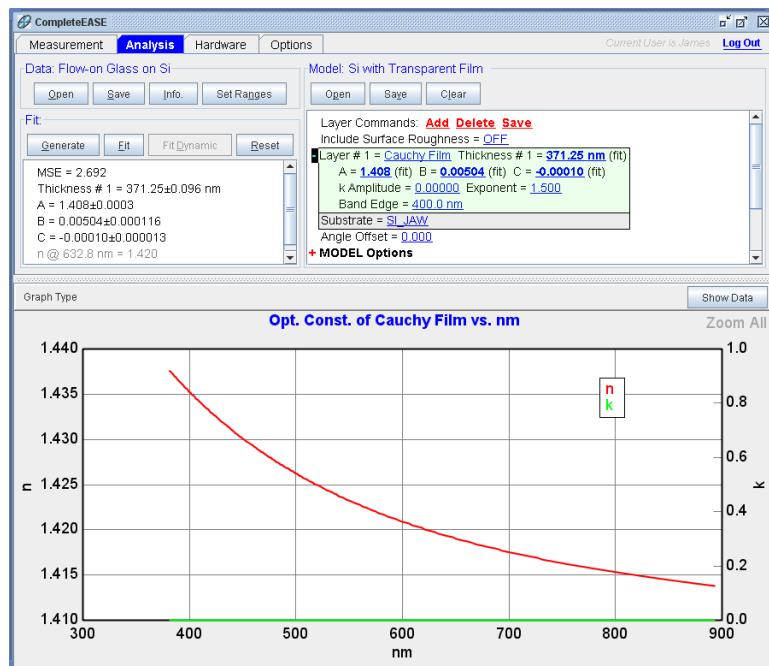


Figure 3-26. Optical constants displayed versus wavelength. Also, the Cauchy layer is expanded, displaying its available fit parameters.

## Global Fits

Like the “Si with Thermal Oxide” model, the “Si with Transparent Film” model uses the “Thickness Pre-Fit” option to provide a good starting value for the layer thickness. To provide starting values for the film index, a “Global” fit is performed. In a Global fit, a wide range of parameter starting values are attempted and the values which result in the lowest MSE are then used as starting values for the “final” fit. The “Use Global Fit” option is found within **Model>+FIT Options**. Turn this option to “ON” to display additional settings which are used to customize the Global fit procedure (Figure 3-27).

In the “Si with Transparent Film” model, the Cauchy “A” parameter for the film (which is basically the approximate index of the film) is defined as a Global fitting parameter. Up to 3 fit parameters can be used in the Global fit. The “Min.” and “Max.” values for “A” are 1.3 and 3.0, and the “# of Guesses” is 30. When the ‘Fit’ button is pressed, the Global fit procedure performs 30 “trial fits” with different starting values for “A”, distributed in equal increments between 1.3 and 3.0. At each trial fit (i.e. for each value of “A” - which corresponds to the film index), a thickness pre-fit is also performed such that the entire array of film thicknesses and indices are attempted. A final fit is performed using starting parameter values from the trial fit which had the lowest MSE.

Layer Commands: [Add](#) [Delete](#) [Save](#)  
 Include Surface Roughness = [OFF](#)

|  |
|--|
| - Layer # 1 = <a href="#">Cauchy Film</a> Thickness # 1 = <a href="#">371.25 nm</a> (fit)            |
| A = <a href="#">1.408</a> (fit) B = <a href="#">0.00504</a> (fit) C = <a href="#">-0.00010</a> (fit) |
| k Amplitude = <a href="#">0.00000</a> Exponent = <a href="#">1.500</a>                               |
| Band Edge = <a href="#">400.0 nm</a>   |
| Substrate = <a href="#">SI_JAW</a>   |
| Angle Offset = <a href="#">0.000</a>   |

+ MODEL Options  
 - FIT Options  
   + Perform Thickness Pre-Fit = [ON](#)  
   - Use Global Fit = [ON](#)  
     # of Data Points = [20](#) # of Iterations = [5](#)  
     Parm #1 = [A](#)  
       Min. = [1.300](#) Max. = [3.000](#) # Guesses = [30](#)  
     Parm #2 = [\(none\)](#)  
     Parm #3 = [\(none\)](#)  
     Include Wvl. Range Expansion Fits = [OFF](#)  
   Fit Weight = [N.C.S](#)  
   Limit Wvl. for Fit = [OFF](#)  
 - Include Derived Parameters = [ON](#)  
   [Add Derived Parameter](#)  
   1: Type = [n](#) Layer # = [1](#) Wavelength = [632.8 nm](#) Name = [n @ 632.8 nm](#)  
     Low Spec. = [0.000](#) High Spec. = [0.000](#)

+ OTHER Options  
[Configure Options](#)  
[Turn Off All Fit Parameters](#)

Figure 3-27. Settings for the “Si with Transparent Film” model; note the “Use Global Fit” and “Include Derived Parameters” sections.

Since the Global fit process is computation intensive, a status bar with a ‘Stop’ button is displayed during the Global fit (Figure 3-28). To speed up the Global fit, only a subset of the experimental data points are used during trial fits based on the “Number of Data Points to Use” option. The number of iterations used in the trial fits can also be limited. The default values for these options (20 and 5) are adequate for most samples, but they can be increased if necessary: larger values may improve the robustness of the global fit, but with the downside of increased analysis time. Likewise, the Min., Max., and # Guesses for the parameter(s) may also need to be “tuned” to handle specific types of samples.



Figure 3-28. Status box and ‘Stop’ button displayed during a Global Fit.

## 3.4. Transparent Substrates

| NEW FEATURES IN THIS EXAMPLE     |                                      |
|----------------------------------|--------------------------------------|
| • Graphing Multiple Data Sets    | • Using the Graph Scratch Pad        |
| • Including Backside Reflections | • Include Depolarization data in Fit |

In the previous example, we introduced the Cauchy dispersion relation to model the index of refraction for transparent films. In addition, the Cauchy can also be applied to transparent substrates. This is the most common approach for substrates of glass or plastic and the “Glass Substrate” model will use a Cauchy to determine the index for glass substrates. This example will demonstrate the modeling of transparent substrates.

With transparent substrates, we must consider a possible complication – the light may reflect from the back surface of substrate and reach the detector. The backside reflections will join the surface reflection, but these two collected beams will be incoherent. This is an optical description for light beams that have lost “phase” information relative to each other. In this case, the backside reflection will only adjust the overall amplitude of the signal and not produce “oscillations” like we see for thin films. This amplitude “offset” from backside reflections can lead to an error in the reported substrate index if not handled correctly. Fortunately, the backside reflections can be corrected in the software (described below).

### Backside Substrate Reflections

The backside reflections that occur with transparent substrates are unwanted. They will affect the measurement and can produce errors in the reported refractive index for either the substrate or the thin films coated on the surface of the substrate. There are multiple ways to deal with transparent substrates and this topic is reviewed by Synowicki<sup>2</sup>. There are two general approaches to deal with transparent substrates. The first is to avoid collection of the backside reflection. Methods to avoid collecting backside reflections include:

- Spatial separation of the backside beam via 1) thick substrate, 2) small measurement beam size, or 3) wedged substrate.
- Scattering and/or absorption of the backside reflection via 1) roughening the backside to scatter light, or 2) applying index-matching material to the backside (cloudy tape has been shown to be successful to this end).

If the backside reflections can not be avoided, then they need to be included in the software calculation. This will be demonstrated during the example. Fortunately, most Woollam SE systems collect depolarization data, which provides evidence of whether backside reflections are present in the collected data. If the depolarization is essentially zero, then no backside reflections reached the detector. This is the preferred condition. If backside reflections reach the detector, the CompleteEASE software can incorporate incoherent interference modeling to correct for the situation. Let’s consider data from a glass substrate to better understand this situation.

<sup>2</sup> R.A. Synowicki, “Suppression of Backside Reflections from Transparent Substrates”, *Phys. Stat. Sol. (c)* **5**, No. 5 (2008) 1085-1088.

## Graphing Multiple Data Sets

Open the data file for “glass substrate\_rough” from the Examples location. This measurement was taken on a glass slide which was mechanically roughened on the backside to eliminate any reflected light from the back surface. Next, ( $\text{Ctrl}+\text{R}$ ) on **Data** > ‘Open’ to access the “Append Data” command, as seen in Figure 3-29. Choose the “glass substrate\_taped” data file from the Examples location. Repeat these steps to also append the “glass substrate\_smooth” data file.

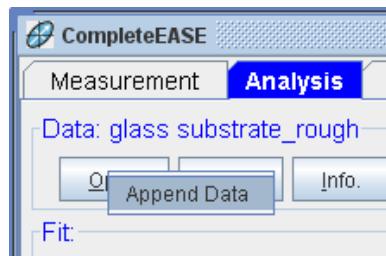


Figure 3-29. ( $\text{Ctrl}+\text{R}$ ) on ‘Open’ command to access the “Append Data” command.

When multiple data sets are appended, CompleteEASE allows all three to be accessed in the Graph window (either individually or the complete set). Select the “Graph Type” command at the top-left of the graph panel and choose to compare Psi. From this same location, also turn off the Double Y Axis. Finally, choose the “Graph All Data Sets” at the top of the Graph panel. This will allow a comparison of the Psi curves collected from all three data sets as shown in Figure 3-30.

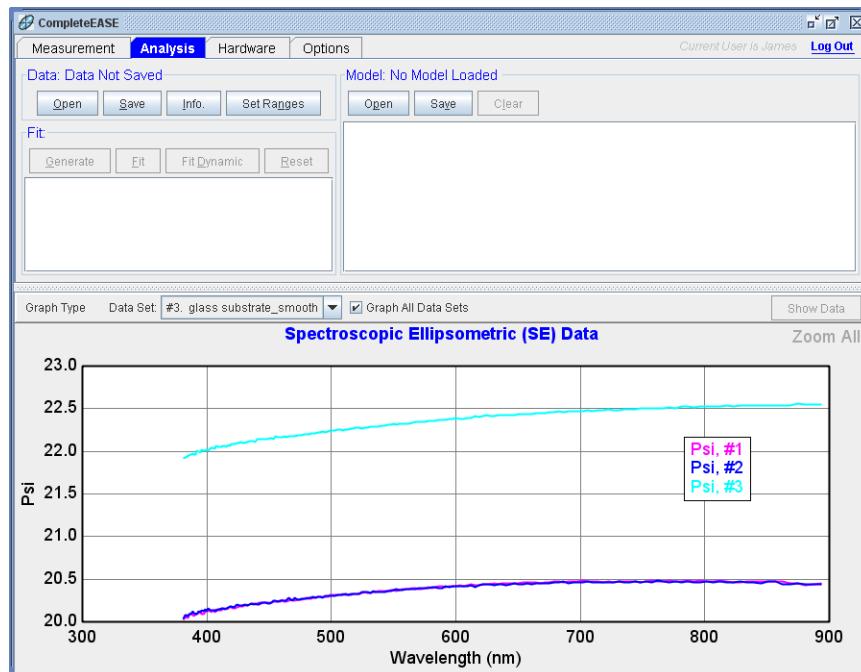


Figure 3-30. When multiple data sets are appended, there are new choices at the top of the Graph Panel to go to any specific data set. Selecting the “Graph All Data Sets” check-box, allows comparisons with all data sets graphed.

## Using the Graph ScratchPad

While the “Graph All Data Sets” provides a quick comparison of the three data sets, it is not customizable. For example, we can’t change the colors or select a subset of the total curves. For this purpose, we turn to the Graph Scratch Pad. Right-click ( $\text{Ctrl}+\text{R}$ ) within the graph area and choose to “Copy Data to Graph ScratchPad”, as shown in Figure 3-31. This will copy all of the curves currently shown on the graph and place them in an internal “pad” for further manipulation. Next, choose to “View Graph ScratchPad” from the same ( $\text{Ctrl}+\text{R}$ ) menu. This opens the CompleteEASE Graph ScratchPad, as shown in Figure 3-32. Play with the ScratchPad by selecting which curves to compare, change their colors, and their styles. Finally, it is beneficial to change their names to correspond to the data set that they came from. Figure 3-33 shows a comparison of the taped and rough glass data – which are nearly identical. This shows that taping the backside can be as effective as roughening the backside of a transparent substrate for removing backside reflections. The data comparison also shows a large difference between the rough or taped data and the data with smooth backside. This large offset is caused by the light reflecting from the backside of the substrate. Next, we will model each data set to show how this backside reflection can produce error in refractive index measurement and finally, how to correct for this backside reflection.

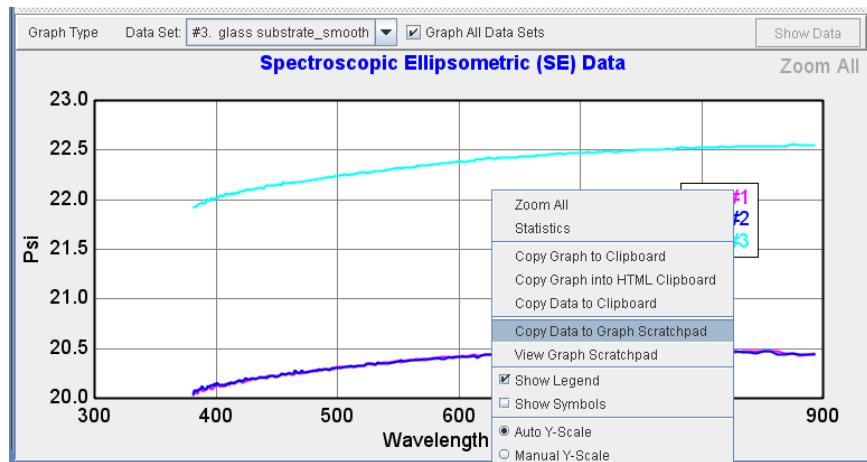


Figure 3-31. Right-click ( $\text{Ctrl}+\text{R}$ ) within the graph area to access the “Graph Scratchpad”.

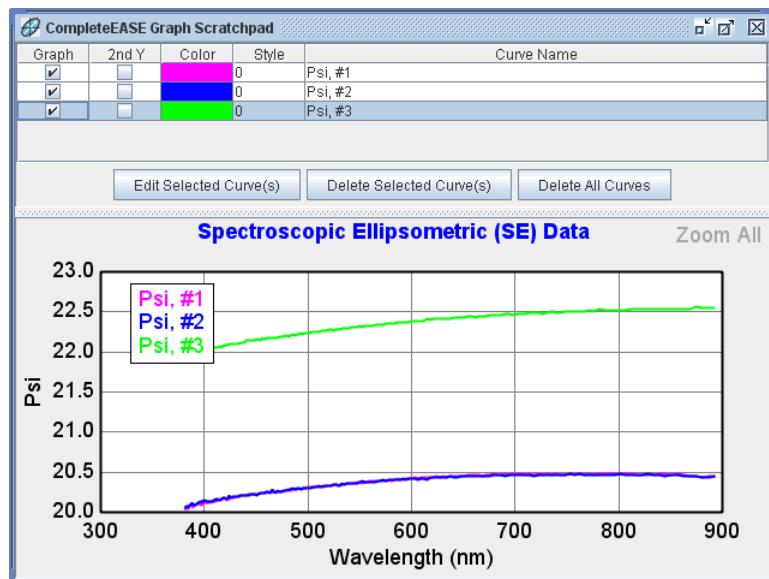


Figure 3-32. CompleteEASE Graph Scratchpad that allows further customization to the graph.

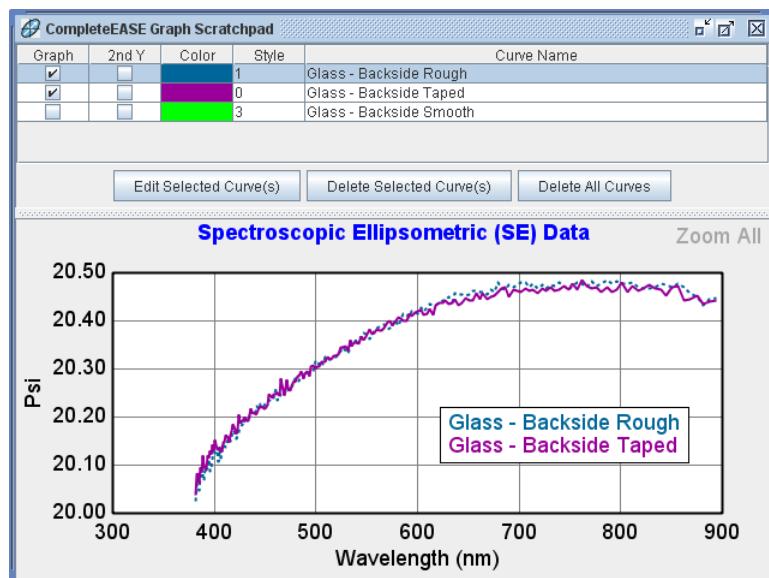


Figure 3-33. The Graph ScratchPad is used to compare data from glass substrate where the backside is roughened or taped to suppress backside reflections.

Before proceeding, clear the contents in the Graph ScratchPad by viewing the ScratchPad and pressing ‘Delete All Curves’.

In a later example, we will learn how to fit multiple data sets simultaneously. However, for this example, we will focus on fitting each individual data set. Start by opening the “glass substrate\_rough” data file. Next, open the “Glass Substrate” model from the Basic folder. Press ‘Fit’ and you should get the result as shown in Figure 3-34. The data appear noisy, but this is primarily due to the graph scale.

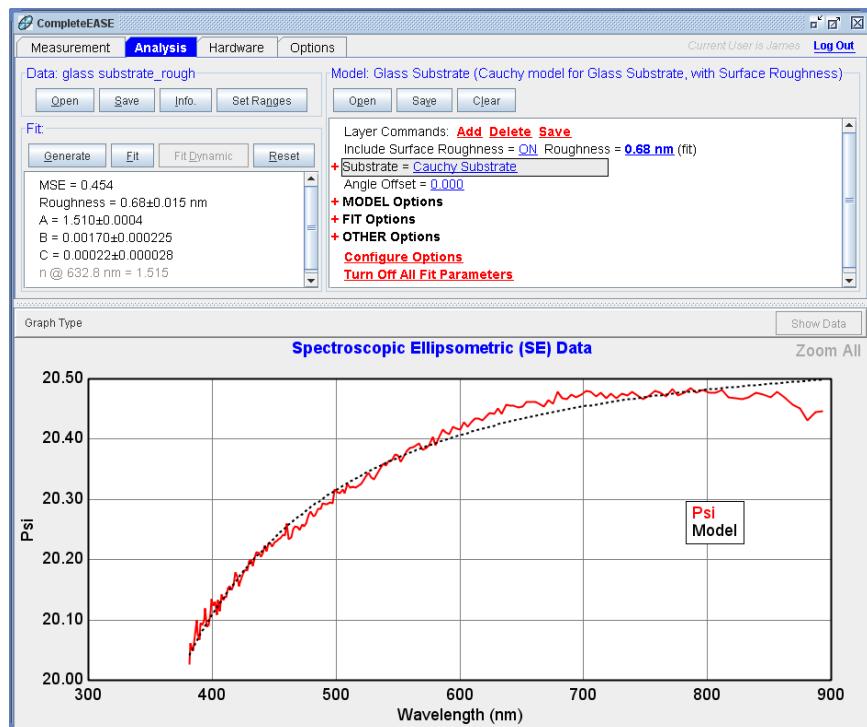


Figure 3-34. Fit to “Glass Substrate” data.

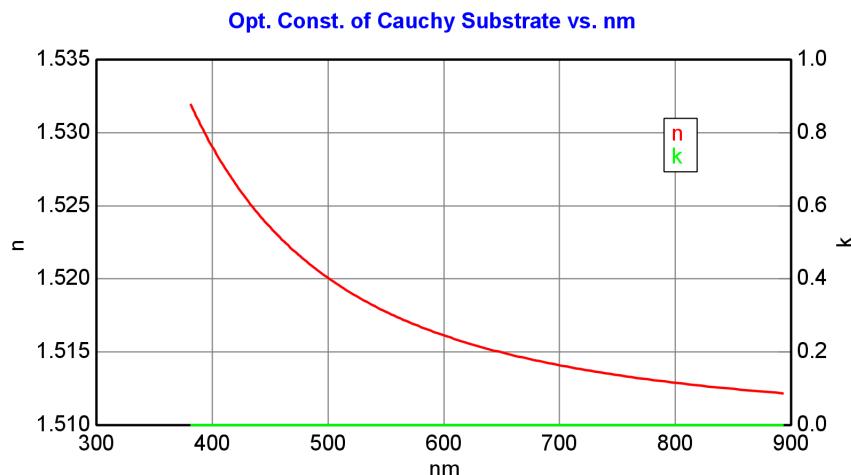


Figure 3-35. Index of refraction from Cauchy model fit to bare glass substrate.

The final index of refraction can be viewed by right-clicking on the Cauchy Substrate and choosing “Graph Layer Optical Constants”. Right-click ( $\text{Ctrl}+\text{R}$ ) inside the Graph and choose “Copy Graph to Clipboard” to transfer the graph shown in Figure 3-35 to Word.

NOTE: Please copy the optical constants graph to the “Graph ScratchPad” before proceeding as we will compare the results to future fits in this example.

## Graphing Depolarization

Ellipsometry measurements use polarized light. If the sample is isotropic and ideal, this measurement can be described by two values:  $\Psi$  and  $\Delta$ . However, if a sample is partially depolarizing, two parameters are insufficient to fully describe the change in polarization. The patented Rotating Compensator technology used in the alpha-SE, M-2000, and RC2 systems permits measurements of three reported quantities:  $\Psi$ ,  $\Delta$ , and %depolarization. The “%depolarization” should remain zero for ideal sample conditions.

HINT: Some ellipsometers require DC measurement to acquire accurate depolarization data. Please consult your hardware manual (or contact JAWCo) to best measure the depolarization.

*Shortcut:*

*CTRL-Z to graph  
Depolarization*

Before proceeding, press on “Graph Type” at the top-left of the Graph. Change from “Psi & Delta” to “Depolarization”. Notice, the Depolarization graph in Figure 3-36 is near zero. This indicates that little light is reflected from the backside into the detector.

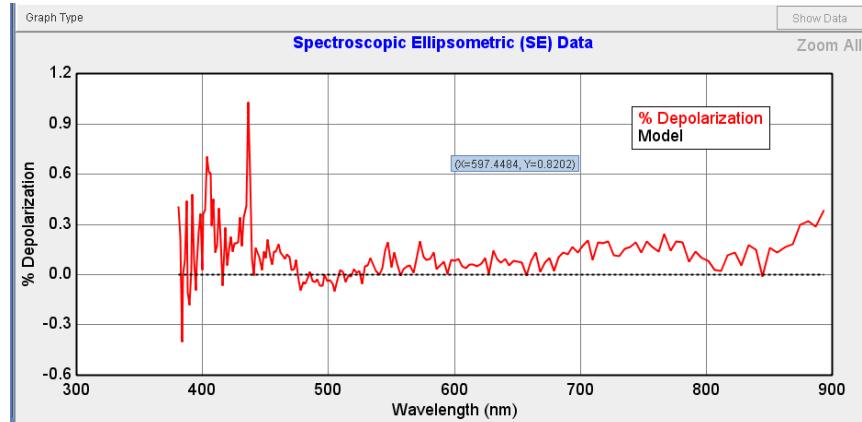


Figure 3-36. Depolarization from uncoated glass slide (no backside reflections).

*Shortcut:*

*CTRL-P to graph  
Psi and Delta.*

Next, open the “glass substrate\_smooth” data file. The graph of Depolarization is now centered at almost 2%. This indicates the backside was smooth and incoherent reflections from the smooth backsurface reached the detector unit. Change the Graph Data back to “Psi”. Press Fit:>‘Generate’. The model no longer matches the experimental measurement even though this data is from the same glass substrate (only with backside reflections). The backside reflections do more than introduce depolarization – they also shift the ellipsometry values. Fit the data with the same model and you should get results as shown in Figure 3-37.

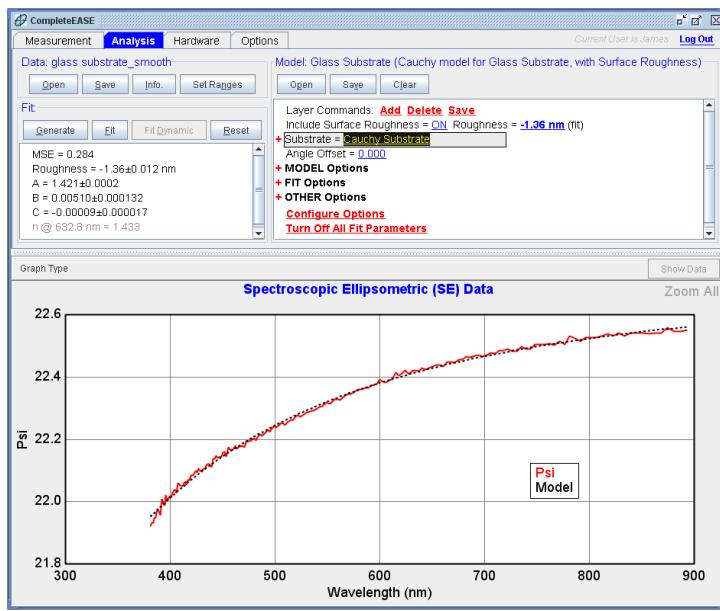


Figure 3-37. Fit results and optical constants for glass substrate\_smooth data modeled without backside reflections.

Before proceeding, view the optical constants and add these new results to the Graph ScratchPad - allowing comparison of the two results in the ScratchPad as shown in Figure 3-38. The first fit result should be correct, as the glass did not include backside reflections. The second fit, with a much lower index of refraction is incorrect because the backside reflections were present in the data, but were not considered in the model. Fortunately, there is a method that can account for backside reflections in measured data and help get correct results. This is considered in the following section as it is a common occurrence with transparent substrates.

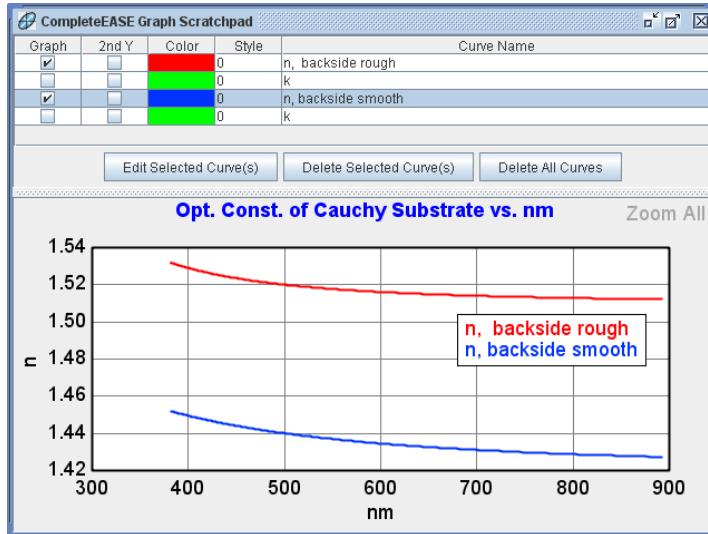


Figure 3-38. Comparison of fit results for refractive index from within the CompleteEASE Graph ScratchPad.

## Including Backside reflections

Backside reflections are common with transparent substrates. Substrates are generally thicker than the coherence length for the white light source of the ellipsometer. Thus, the returning light does not interfere in a coherent sense, as its phase information is lost compared to the reflections from the top-surface coatings.

Back-side reflections are undesirable when characterizing surface films. This is especially true if the substrate is anisotropic. To prevent back-side reflections the back-surface can be roughened to scatter light, as in Figure 3-39. For thicker substrates, the backside reflections may be spatially separated at the detector and thus not a concern.

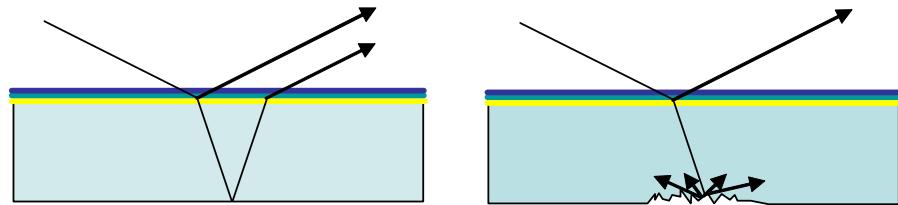


Figure 3-39. Reflections from the backsurface of transparent substrate are incoherent. This light can be avoided by roughening the backsurface to scatter the reflected light.

If the backside reflections can't be avoided, the "incoherent" summation of light beams can be handled mathematically. To include backside effects in the model, expand the **+MODEL Options** section of the Model. Turn "Include Substrate Backside Corrections" to ON, as shown in Figure 3-40. The correction depends on the amount of light collected from the backside, which can differ for different substrates. In the Model Options section, select the "# Back Reflections" as a fit parameter.

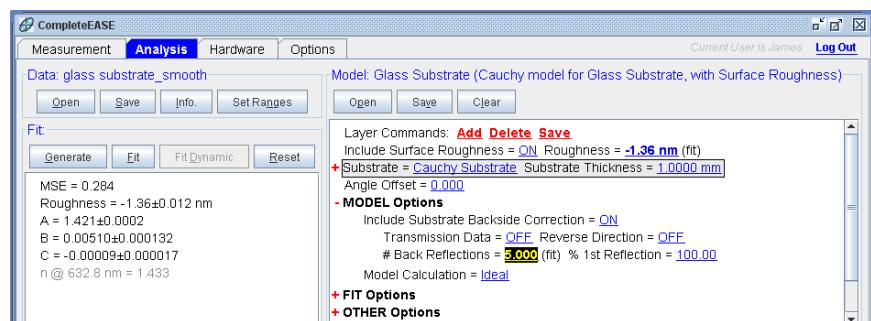


Figure 3-40. Model Options expand to allow Include Substrate Backside Correction. The number of Back Reflections can be "fit" to best match the experimental data.

## Fitting Depolarization

There is correlation between the substrate index and the amount of backside light collected when modeling ellipsometry data at one angle of incidence. However, depolarization data is only influenced by the amount of backside light collected. The default setting is to ignore the depolarization data and only fit Psi and Delta. In fact, the depolarization fitting selection is a hidden feature of the model. To show this feature, go to the bottom of the **Model:** pane and press [Configure Options](#). This

will bring up the dialog box shown in Figure 3-41. Check the box next to “Include Depolarization Data” in the Fit Options section and then ‘Ok’. With this option shown, choose **Model:>+Fit Options** and turn the “Include Depolarization Data” to ON, as shown in Figure 3-42.

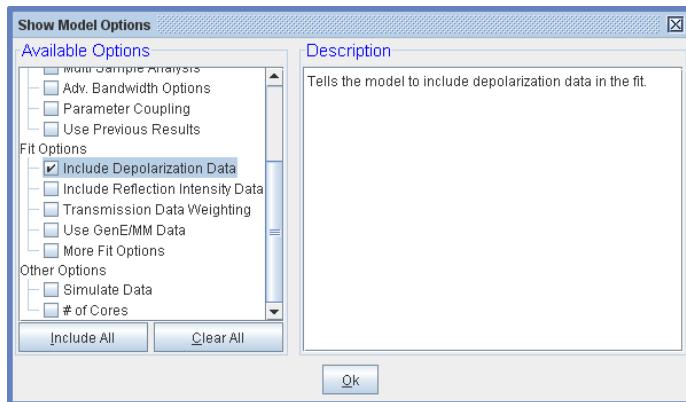


Figure 3-41. Press **Configure Options** to show additional Model options. In this example, we will add “Include Depolarization Data” as shown.

#### + MODEL Options

##### - FIT Options

Perform Thickness Pre-Fit = OFF

Use Global Fit = OFF

Fit Weight = N.C.S

Include Depolarization Data = ON % Weight = 100.00

Limit Wvl. for Fit = OFF

+ Include Derived Parameters = ON

##### + OTHER Options

Figure 3-42. The “Use Depol. Data in Fit” selection within the Fit Options section of model.

Press ‘Fit’ again for the “Glass Substrate\_smooth” data including the backside reflections (with fit to # of Back Reflections collected) and using the Depolarization data in fit. You will probably have to reduce the # of Backside Reflections down to 1 (from default of 5) to get the depolarization data to fit. When done correctly, the result should appear as in Figure 3-43. The measurement of depolarization provides sensitivity to the amount of backside reflected light that is reaching the detector. In this case, the best fit is with 1.5 backside reflections, as shown in Figure 3-44 (where the number of backside reflections is varied to see whether the number of backside reflections is a unique result). This means the substrate is thin enough that the first reflection from backside is completely collected in the detector, while the second reflection is spatially shifted enough to only collect about half of this second reflection. Of course, as the number of reflections increases, the amount of additional light reaching the detector is much lower and the sensitivity goes down. Thus, there is little difference in the calculation between 3, 4, and 5 total reflections from the backside.

Before proceeding, let’s view the optical constants from this result and copy the graph to the Graph ScratchPad for further comparison with our previous results. The final comparison of optical constants is shown in Figure 3-45. The index for backside roughened glass is similar (but not exactly equal) to the results for smooth

backside glass when the fit is corrected including depolarization. If the backside effects are not considered, the fit results significantly affect the index of refraction. There are two possibilities as to the difference in final results when corrected:

- Depolarization data not accurately determined.
- Some backside reflections for roughened glass still remain.

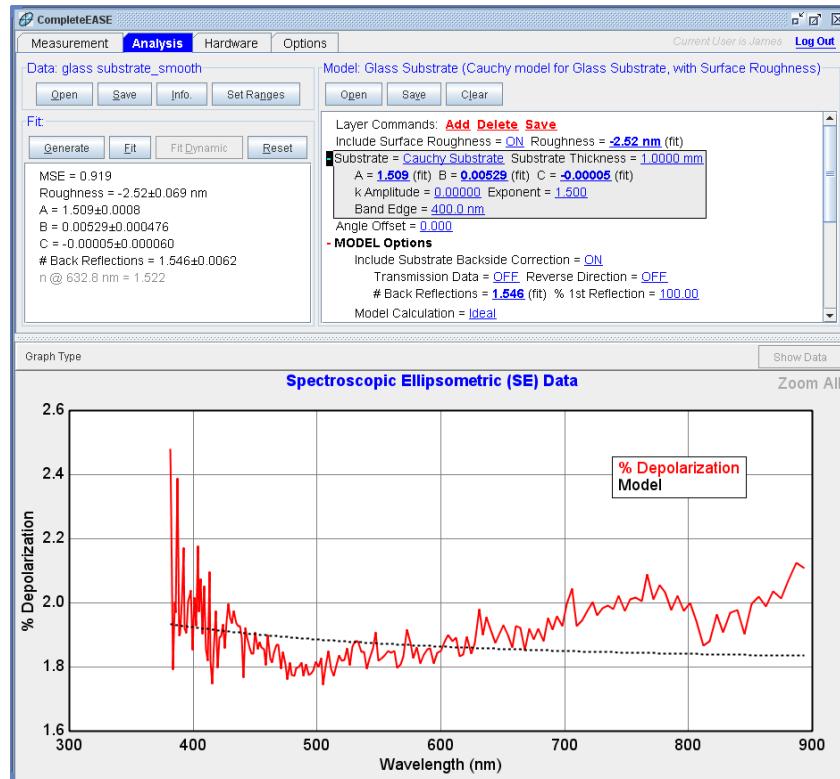


Figure 3-43. Fit results including backside reflections and depolarization data.

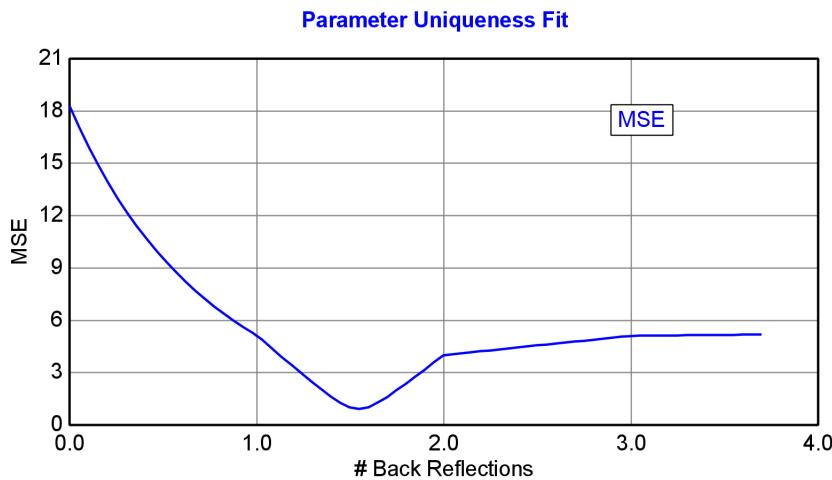


Figure 3-44. Uniqueness Test for the # of Backside Reflections, showing that the best fit results from about 1.5 backside reflections. The depolarization measurement helps to quantify this result.

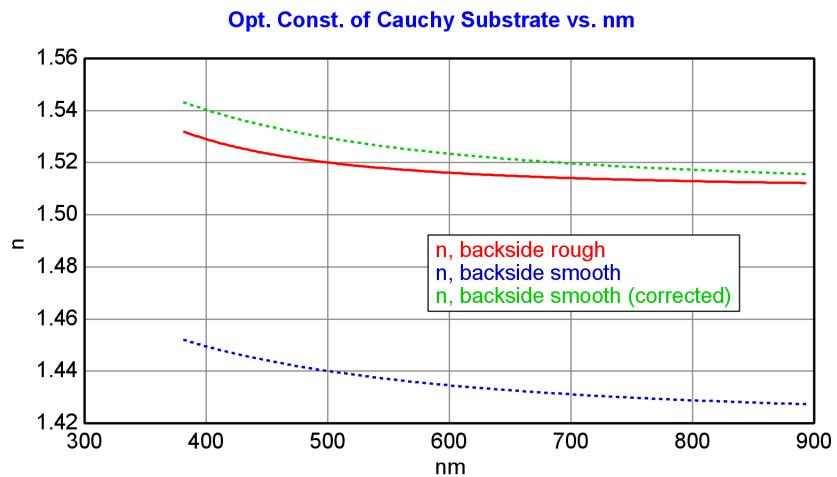


Figure 3-45. Final comparison of glass index results.

## 3.5. Transparent Films - 2

### FEATURES IN THIS EXAMPLE

- Surface Roughness
- Grade Layer
- **Try Alternate Models**

### Glass with Transparent Film

For this example, load the “Glass with Transparent Film” model and the “ZrO<sub>2</sub> on Glass” data file. Click the ‘Fit’ button: a Global fit will be performed and the fit results are displayed as shown in Figure 3-46. The refractive index for the ZrO<sub>2</sub> film can be displayed by right-clicking ( $\text{Ctrl}+\text{R}$ ) on “Cauchy Film” and choosing “Graph Layer Optical Constants. The results are shown in Figure 3-47.

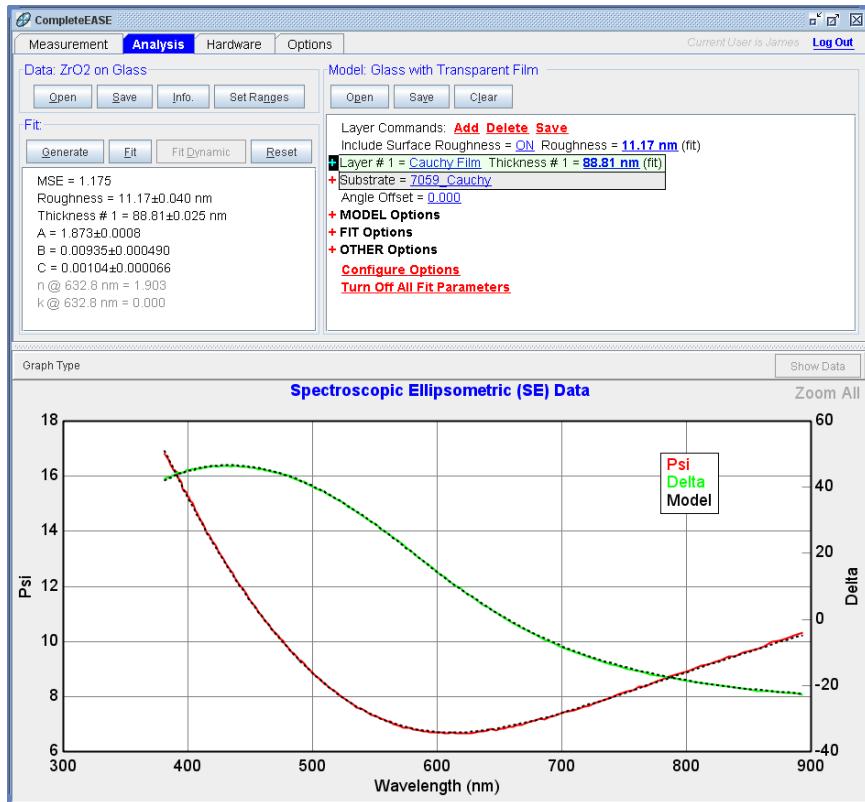


Figure 3-46. Fit results from analysis of “ZrO<sub>2</sub> on Glass” example file, using the “Glass with Transparent Film” model.

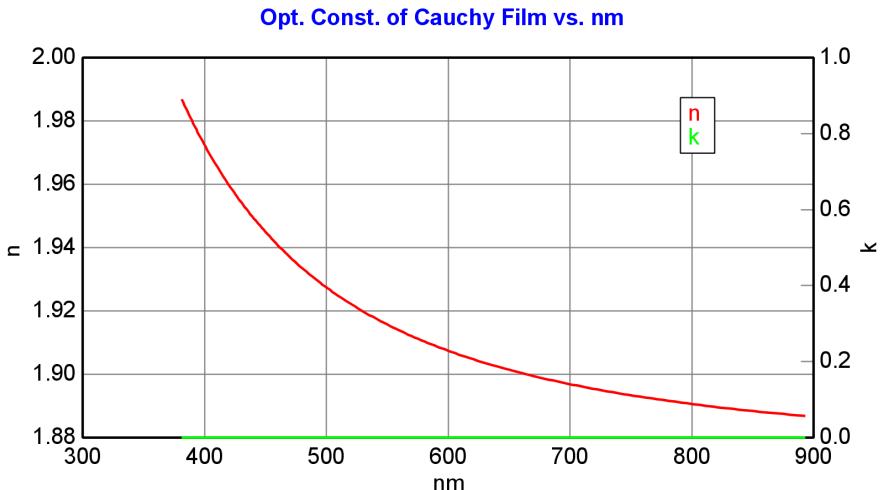


Figure 3-47.  $\text{ZrO}_2$  optical constants from fit using Cauchy dispersion layer.

The main difference between the “Glass with Transparent Film” and the “Si with Transparent Film” model which was used in previous examples is the material file used for the substrate: “7059\_Cauchy” instead of “SI\_JAW”. As the optical constants for 7059 glass are representative of many glass substrates, this model can be used as a starting point for many transparent films on glass. More accurate results could be achieved by replacing the 7059\_Cauchy material with optical constants measured on *your* bare glass substrate (see section 3.4). In addition, because the substrate is transparent, backside reflections may be an issue. To test whether backside reflections are present in this data, press CTRL-Z to view the Depolarization data as shown in Figure 3-48. As the depolarization is centered at zero, it is likely that the backside reflections were suppressed to avoid collection at the detector. These issues are discussed in more detail in Section 3.4.

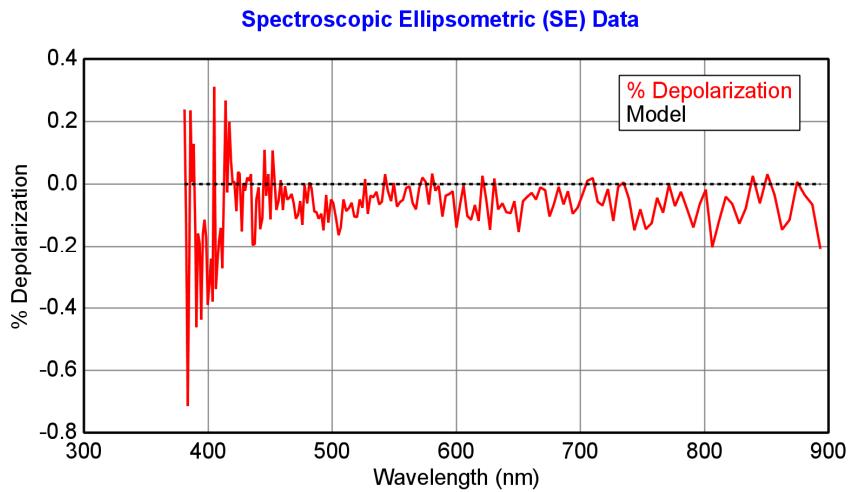


Figure 3-48. Depolarization data is near zero percent, which indicates that backside reflections were not collected even though substrate was transparent.

## Surface Roughness

An interesting feature to the current model is the inclusion of surface roughness (the “Include Surface Roughness” option is set to “ON”). Actually, the best fit surface roughness value for this sample is rather large: 11.17 nm. To test the importance of roughness in this model, try fitting the data **without** surface roughness: toggle the “Include Surface Roughness = ” value to “OFF” by clicking ( $\text{F}\text{L}$ ) on the blue underlined value. Since we already know the nominal thickness and index, it is also wise to turn OFF both the “Use Global Fit” and “Thickness Prefit”. Go ahead and click the ‘Fit’ button, which will fit the data without roughness – resulting in a poor fit and higher MSE, as displayed in Figure 3-49.

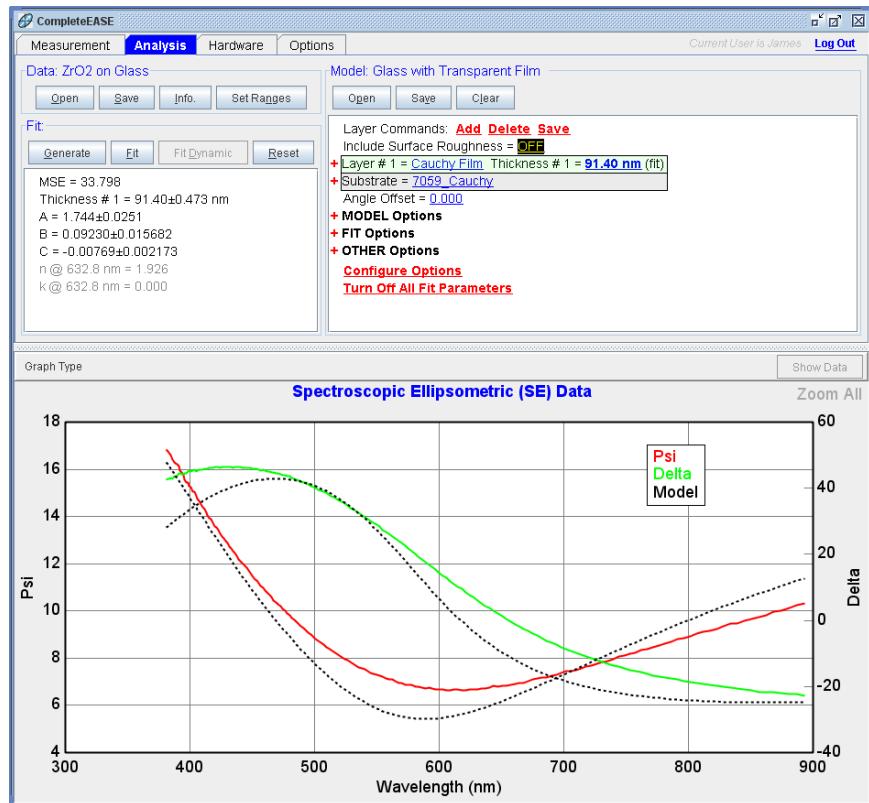


Figure 3-49. Fit to “ZrO<sub>2</sub> on Glass” data with surface roughness OFF.

## Graded Index

Surface roughness, which is one of the model “non-idealities” discussed in section 3.1, is very important to achieve a good model fit on this sample. Another non-ideality described in section 3.1 is index grading. With the surface roughness turned off, try grading the film as described below:

- ( $\text{C}\text{R}$ ) on the name “Cauchy Film” of Layer #1. You should see a drop-down menu, as shown in Figure 3-50. Choose “Grade Layer”.
- The “% Inhomogeneity” and Thickness are defined as fit parameter.
- Press ‘Fit’ and the results will appear as in Figure 3-51.

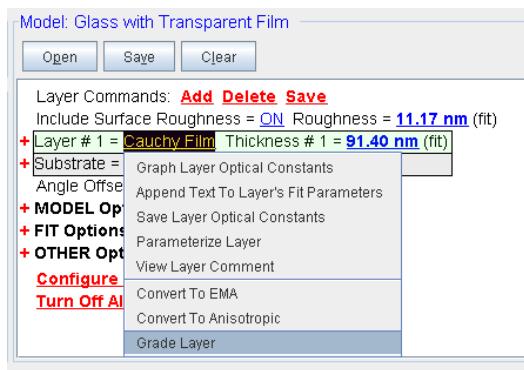


Figure 3-50. Right-click on Cauchy Film to access drop-down menu, then choose to Grade Layer.

**NOTE:** Surface roughness and index grading often have the same effect on modeled data, as they can both reduce the optical density of a material toward the surface. If both give similar MSE values, it is up to the user to judge which is best for their sample.

While the fit appears quite good to the eye, the MSE is slightly higher than for the model which included surface roughness (2.1 vs. 1.175).

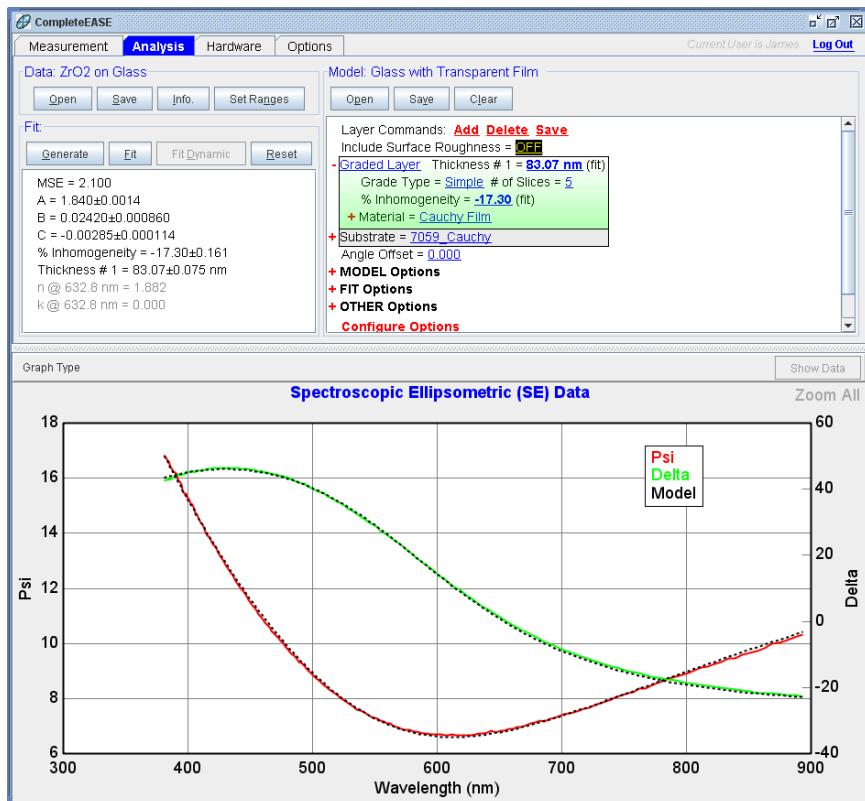


Figure 3-51. Fit to “ZrO<sub>2</sub> on Glass” data with index Grading ON.

It is also possible to combine surface roughness and index Grading in the model: turn the surface roughness back “ON” and press ‘Fit’ (leaving the “% Inhomogeneity” defined as a fit parameter). The results shown in Figure 3-52 indicate this model yields the lowest MSE yet (0.78).

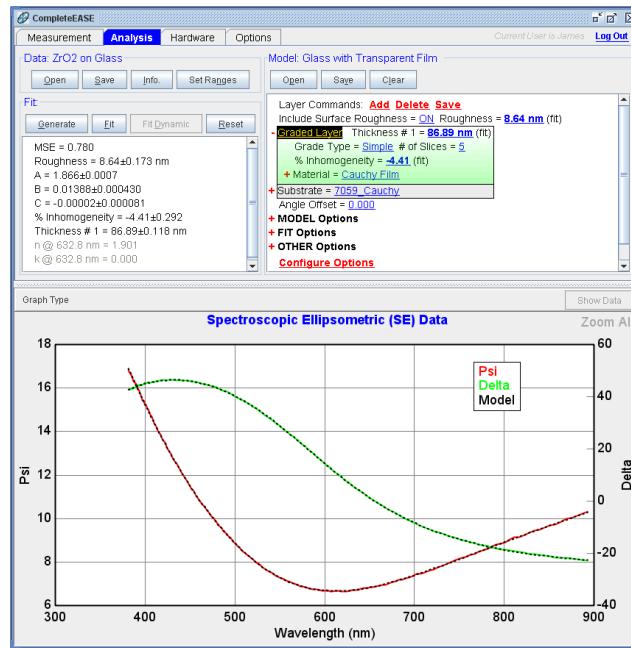


Figure 3-52. Fit results for “ZrO<sub>2</sub> on Glass” data fit with model that includes both surface roughness and grading.

## Try Alternate Models

NOTE: This command will not work if the film is already graded. To remove grading from our current model, ( $\text{Ctrl}+\text{R}$ ) on Graded Layer and select “Remove Grading”, as shown in Figure 3-53.

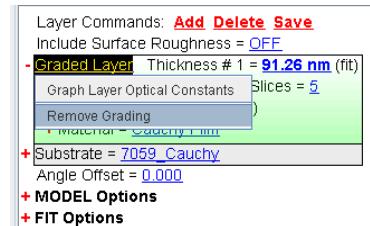


Figure 3-53. Remove Grading by right-clicking on the Graded Layer name and then select “Remove Grading”.

The process of trying optical models with and without surface roughness and index grading is so common in SE data analysis that CompleteEASE has a command to automate the procedure. Once a good starting model is established, click **Model>+OTHER Options>Try Alternate Models**, as shown in Figure 3-54. Fits will automatically perform with the ideal optical model, with surface roughness, with index grading, and with roughness & grading. Fit results are summarized in tabulated and graphical formats, as shown Figure 3-55. The highlighted “green” column is a suggestion of the “best” optical model, based on 25% improvement in MSE for each additional fit parameter.

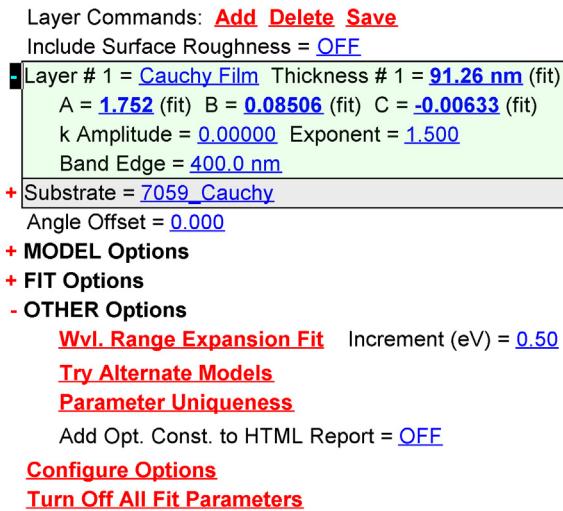


Figure 3-54. Model panel with the +OTHER Options section expanded to show the [Try Alternate Models](#) option.

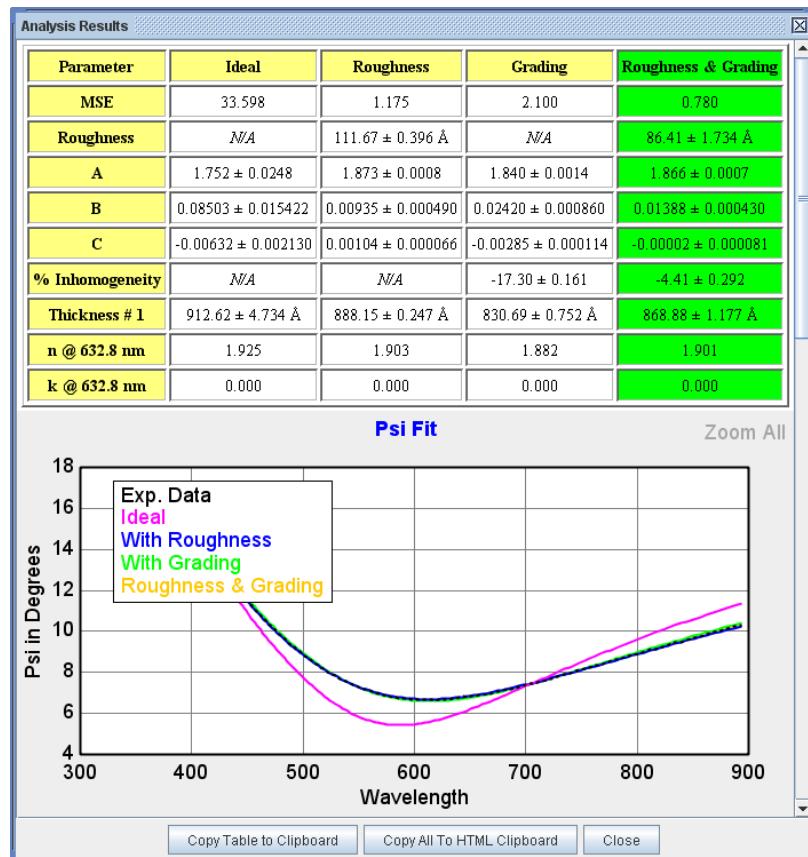


Figure 3-55. Results of the [Try Alternate Models](#) command.

## 3.6. Log and Report a Series of Films

| FEATURES IN THIS EXAMPLE   |  |
|--|--|
| <ul style="list-style-type: none"><li>• Copying to Clipboard</li><li>• HTML Clipboard</li><li>• Fit Log</li><li>• Save/Open Snapshot</li></ul> | <ul style="list-style-type: none"><li>• Comparing Optical Constants</li><li>• Creating a Report</li><li>• Re-analyzing data from log</li></ul> |

One of the most common applications of any ellipsometer involves measurement of a series of thin films, which are to be compared and reported. The CompleteEASE software enables simple logging, comparing, and reporting of results. This example will step through a series of SiNx thin films on Silicon, using the analysis steps taught in Section 3.3. However, the emphasis will be on using CompleteEASE to log all fit results, compare optical constants for the various films, and finally create a record (or report) of the results.

To begin this exercise, open “SiNx on Si-1” data file and the “Si with Transparent Film” model in the **Analysis** tab of CompleteEASE. Go ahead and press ‘Fit’ and the results shown in Figure 3-56 appear.

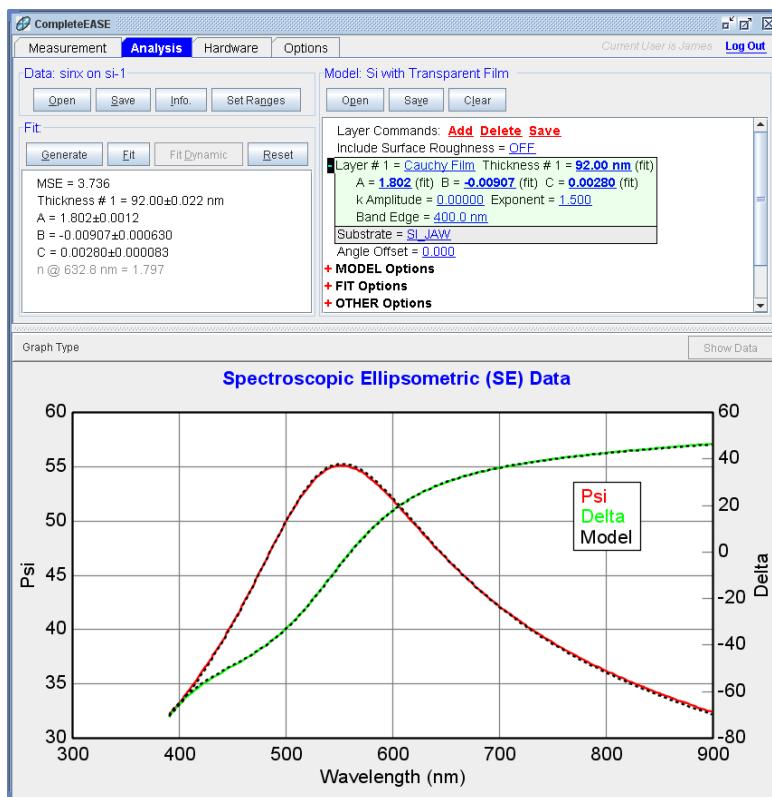


Figure 3-56. Fit to “SiNx on Si-1” data file using “Si with Transparent Film” model.

## Copy to Clipboard

Each pane (white area) in the **Analysis** tab of CompleteEASE offers right-click (**CTRL+R**) menu choices. Examples of these right-click menus are shown in Figure 3-57. In addition, the Graph also features a right-click menu, as shown in Figure 3-58. To assist in creating reports, the model, fit results, and various graphs can be copied to the clipboard and then pasted in various programs such as Word, Excel, or PowerPoint. The Fit results can be copied to the clipboard using Formatted or Table choices, where the former is best for pasting into a word processor and the latter is preferred for pasting into a spreadsheet. The Model can be copied in its entirety or as the layers only.

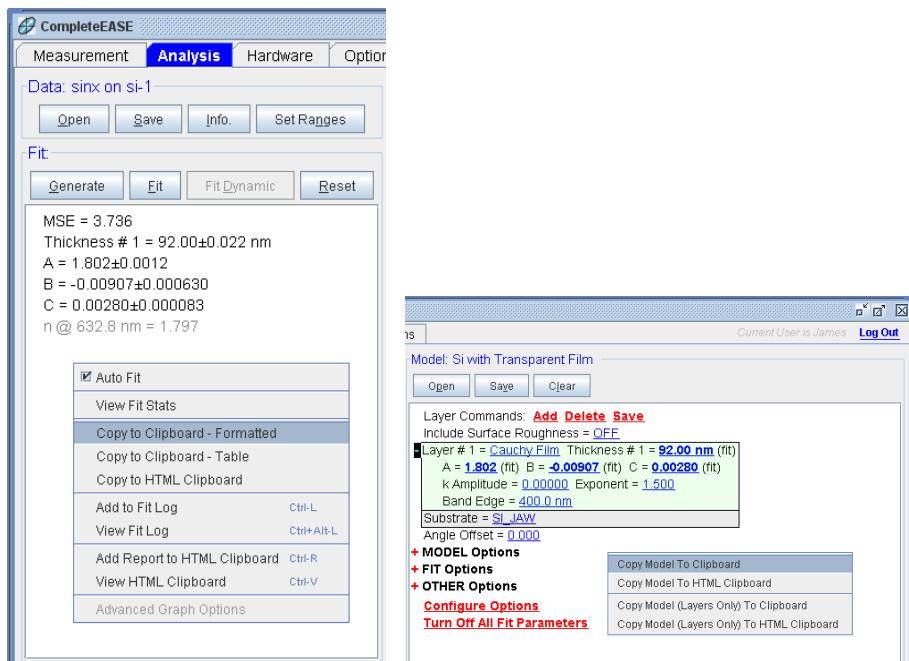


Figure 3-57. Right-click (**CTRL+R**) menu choices from the **Fit:** and **Model:** panes.

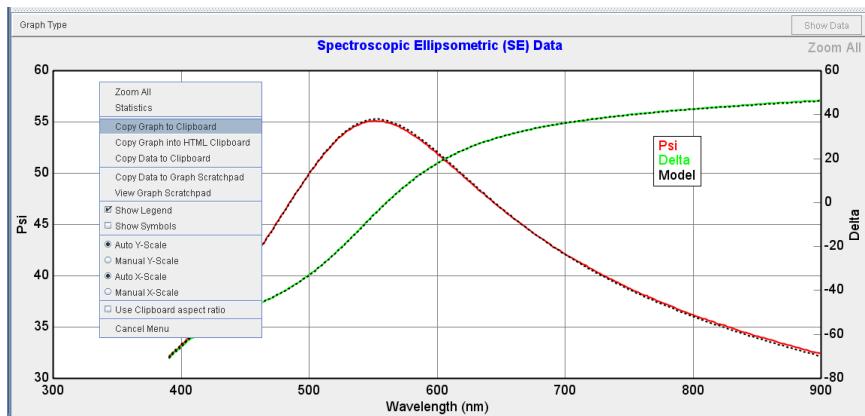


Figure 3-58. Right-click (**CTRL+R**) menu choices from the Graph.

## HTML Clipboard

In addition to the standard clipboard, there is a choice from Model, Fit Results and Graph to use the HTML clipboard. This is a special area that can be used to create a report and then later copy in its entirety to a separate document. In addition, CompleteEASE has a “quick” report that can be automatically created from the **Fit:** panel. After you have finished analyzing a sample, such as the SiNx film that we are currently working with, press the **(CTRL-R)** from the **Fit:** panel and choose “Add Report to HTML Clipboard”. Alternatively, you can press CTRL-R to achieve the same function. After copying the “Report” into the HTML clipboard, press CTRL-V to view the HTML report (or access the right-click menu again and choose “View HTML Clipboard”). The clipboard will contain fit results, model and graph in a self-contained report, as in Figure 3-59.

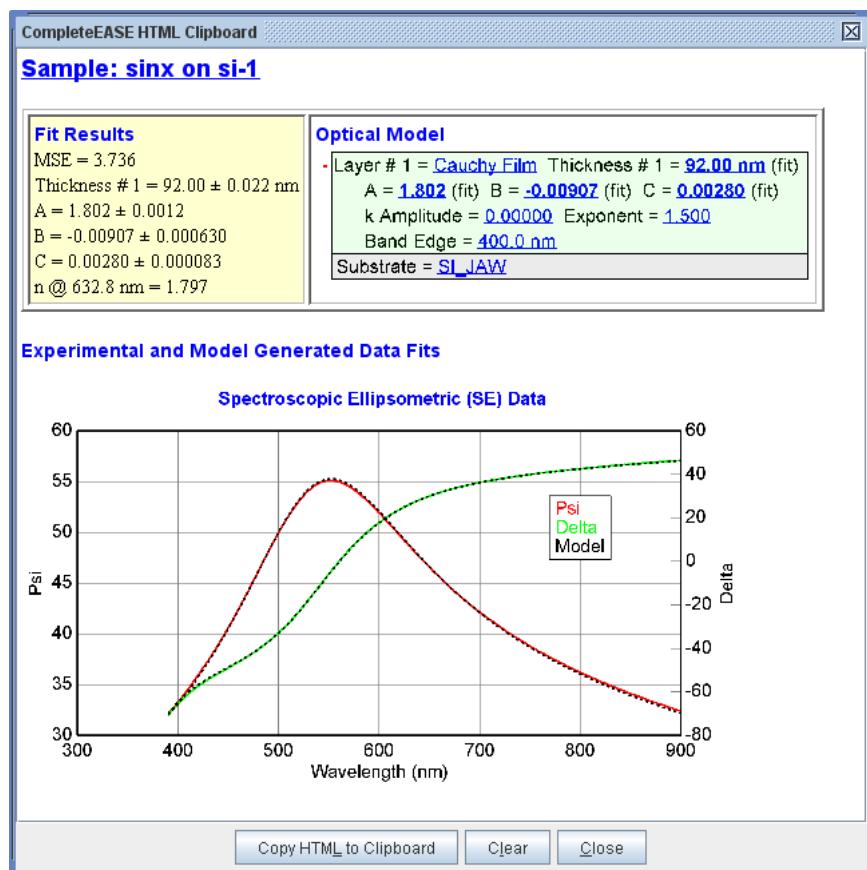


Figure 3-59. CompleteEASE report created in the HTML clipboard.

## Fit Log

Now, work through all five SiNx on Si samples in the Examples folder. To record the final fit results for each film, right-click **(CTRL-R)** on the **Fit:** pane and “Add to Fit Log” after the fit is finished. This will save the current fit results. Type in an appropriate name for each fit result.

The short-cut key to add results to the Fit Log is CTRL-L.

After all five data files have been fit and added to the Fit Log; choose to “View Fit Log” from the right-click (**CTRL-R**) menu of the **Fit:** pane. This should bring up a Fit Log with each of the five entries, as in Figure 3-60. You can press on any of the individual log entries to see the results from that sample.

The short-cut key to View the Fit Log is CTRL-ALT-L.

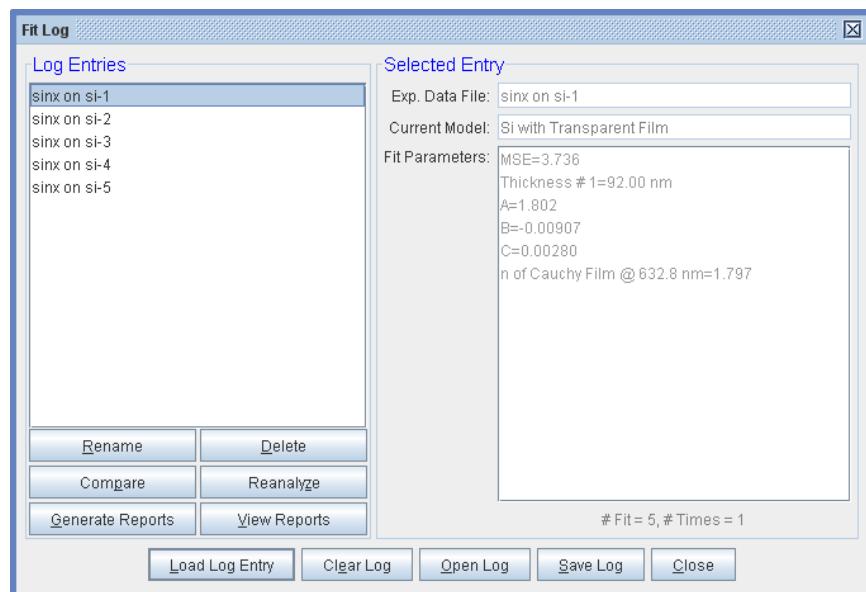


Figure 3-60. Fit Log showing results from all five SiNx on Si data files.

## Comparing Results

Now, select all five Log Entries by selecting the first entry with your mouse and then holding the shift-key down while you press the last Log entry. With multiple Log entries selected, press the ‘Compare’ button. This will create a Table of results for each sample, as in Figure 3-61. The columns/rows can be reversed by a simple button click. Also, the statistics can be added with a click. This table can be conveniently copied to the clipboard.

The screenshot shows the 'Comparison' dialog box. It contains a table titled 'Entry Comparison Table' with the following data:

|              | MSE   | Thickness # 1 (nm) | A     | B        | C       | n of Cauchy Film @ 632.8 nm |
|--------------|-------|--------------------|-------|----------|---------|-----------------------------|
| sinx on si-1 | 3.736 | 92.00              | 1.802 | -0.00907 | 0.00280 | 1.797                       |
| sinx on si-2 | 2.651 | 101.28             | 1.735 | -0.00044 | 0.00149 | 1.743                       |
| sinx on si-3 | 2.837 | 96.71              | 1.858 | -0.00426 | 0.00280 | 1.865                       |
| sinx on si-4 | 3.210 | 87.61              | 1.916 | -0.00298 | 0.00281 | 1.926                       |
| sinx on si-5 | 2.516 | 105.48             | 1.804 | -0.00032 | 0.00203 | 1.816                       |

At the bottom of the dialog, there are buttons for 'Reverse Columns/Rows', 'Add Statistics', 'Copy To Clipboard', 'Close', and 'Compare Optical Constants'.

Figure 3-61. Comparison Table showing results from all five SiNx films.

## Compare Optical Constants

From the Comparison Table, press the ‘Compare Optical Constants’ button and dialog box appears as in Figure 3-62. Select each of the layers you would like to compare and choose the type of graph and you can compare the index for each of the SiNx layers, as shown in Figure 3-63. This graph can be conveniently copied to the clipboard or to the HTML clipboard to be added to the report.

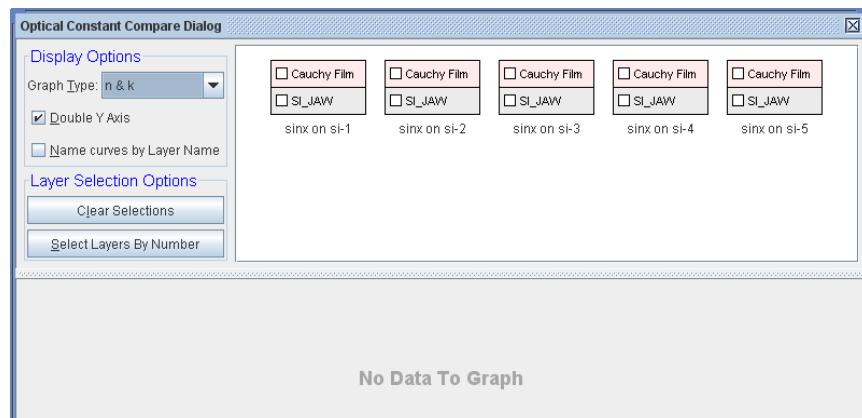


Figure 3-62. Compare Optical Constants Dialog Box.

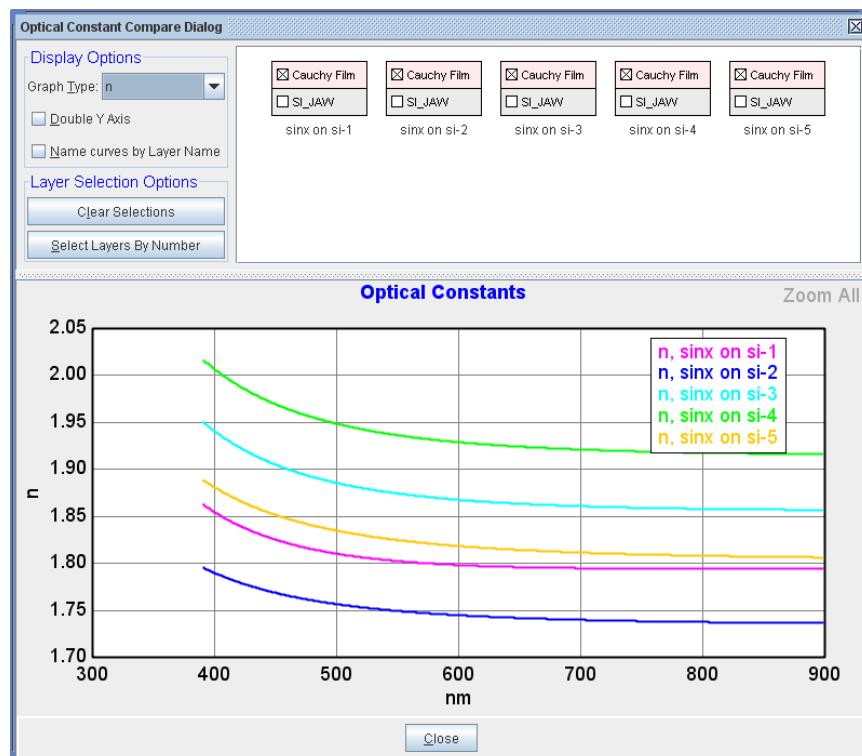


Figure 3-63. Choose the layers to compare and the type of graph.

## Re-analyzing Multiple Data Sets

The process we just finished for the series of SiNx samples is quick, but somewhat repetitive. In this fortunate case where all samples can be analyzed with a single model, there is a much faster way to analyze the data and build a master report.

First, clear the Fit Log and the HTML clipboard from our previous efforts. To clear the HTML clipboard, press CTRL-V to view the HTML clipboard and press ‘Clear’ button at the bottom. To clear the Fit Log, press CTRL-ALT-L to view the Fit Log and press the ‘Clear Log’ button. Now, you are ready to repeat this example using a faster, easier method.

To start, press CTRL-ALT-L to view the Fit Log. There should be no current entries, as we just finished clearing the log. Press the ‘ReAnalyze’ button, which will open the dialog window as shown in Figure 3-64. Select “Choose Files Manually” and you will be asked which files to analyze. Select all five SiNx data files that we just recently analyzed. Next, press “Choose a Model” and select the “Silicon with Transparent Film” model that we used for these nitride films previously. Go ahead and press ‘Reanalyze’. This will run through the analysis of all five data files and save the results of each to the Fit Log. This one step has reproduced the entire example we worked earlier in this section.

Note: The “Re-save Data” check-box allows the new fit results to be saved along with each data file.

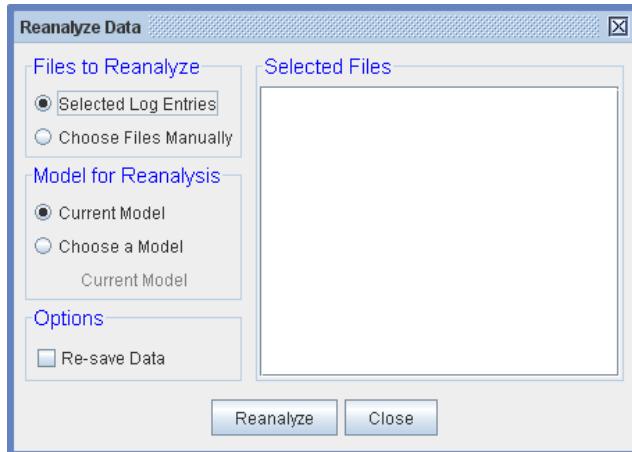


Figure 3-64. ReAnalyze Data window opened from within the Fit Log.

## ‘Generate Report’

Now, use another one-step approach to create a report for all the results. View the Fit Log (CTRL-ALT-L) and select all five entries. Next, press the ‘Generate Reports’ button, as shown in Figure 3-65. This copies the results of each log entry into the HTML Clipboard. When finished, press the ‘View Reports’ button to view the HTML clipboard, as seen in Figure 3-66.

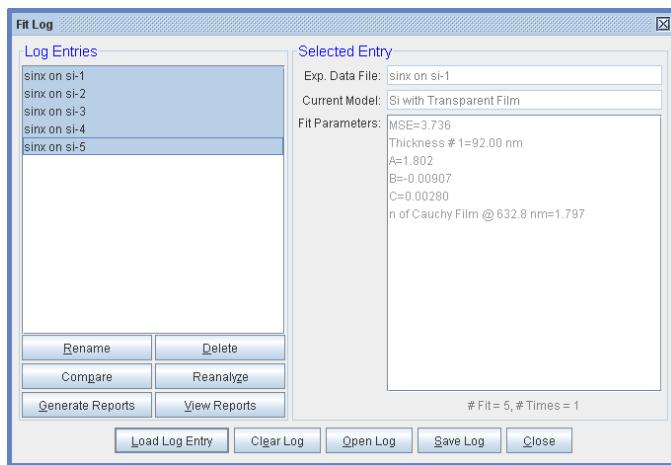


Figure 3-65. All log entries are selected and the 'Generate Reports' button is pressed to copy all results into the HTML Clipboard.

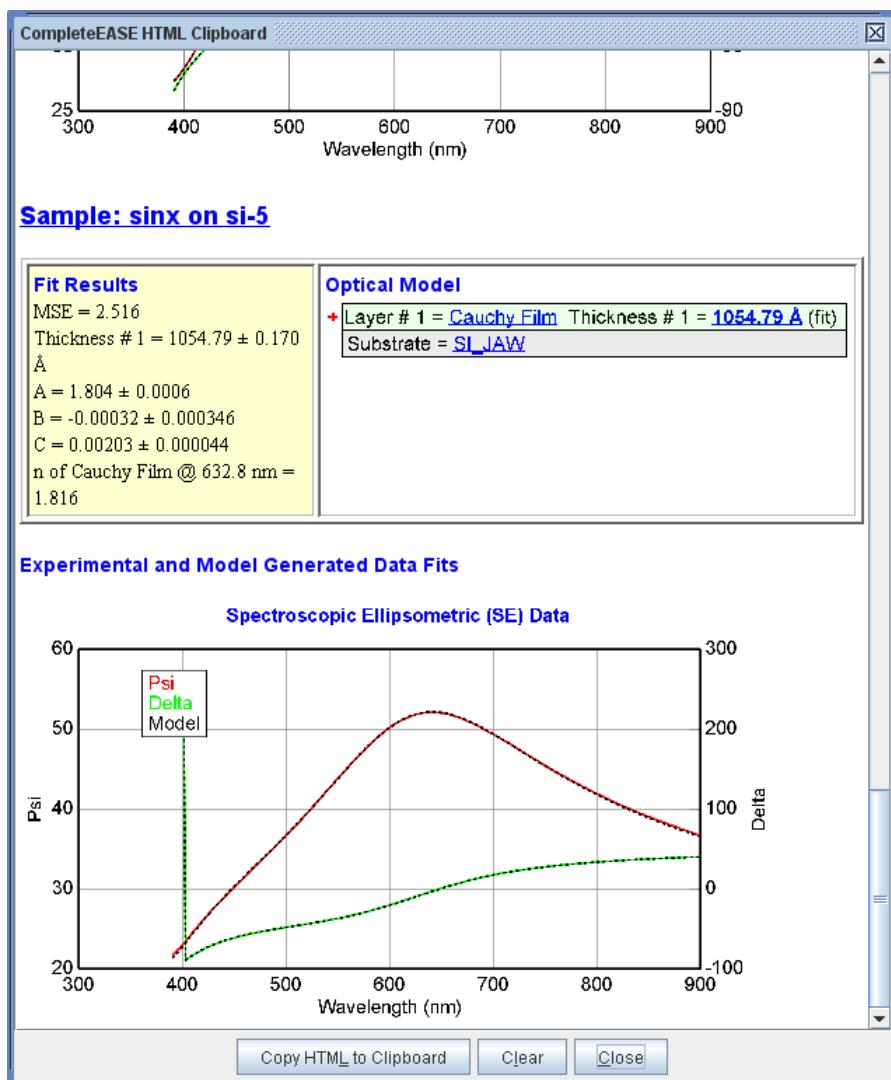


Figure 3-66. HTML Clipboard after a report has been generated for all entries in the Fit Log.

## Save Log File

When finished with a project, you may want to save the results or send them to a colleague. The Fit Log is a nice way to store all of the modeling results you have completed. You can save a Fit Log, by selecting “View Fit Log” from the **Fit:** panel right-click menu. Then, choose the ‘Save Log’ button, as shown in Figure 3-60. The log will be saved with a “fit” extension. The log will include the list of all entries, with the filename for each data file needed and the model layers. To open the log, the data files must be in the same directory as the “fit” log file. Thus, if you intend to send your log to a colleague, they will also need all of the Data files to open the log file.

## Snapshot

A better way to send single fits to a colleague, or save them for future use, is to save the Snapshot of your fit result. A snapshot will compress your data file, model, and fit results into a single file with “SS” extension. Thus, a single snapshot file can be stored or sent and then opened to get back to the same result that you saved. To save a Snapshot after performing a Fit on a SiNx data example, simply right-click your mouse over the Model:> ‘Save’ button, as shown in Figure 3-67. To open the Snapshot, simply right-click your mouse over the ‘Open’ button above the model.

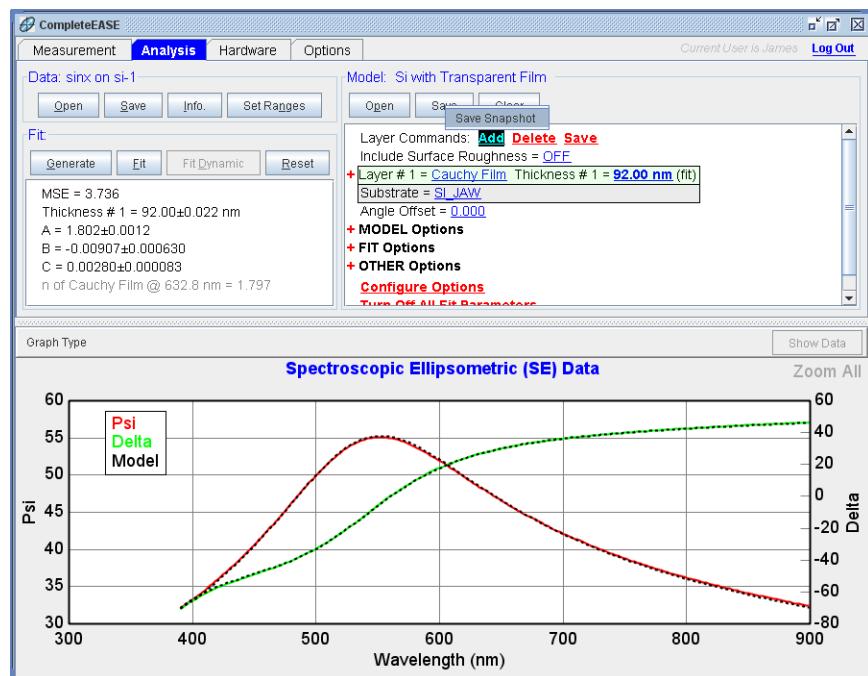


Figure 3-67. Save a Snapshot of your result by right-clicking mouse button over the ‘Save’ button in the **Model:** panel.

# 4. Data Analysis 2 - Intermediate

This chapter continues the series of examples with intermediate concepts, concentrating on absorbing materials. The section examples from this chapter are listed below, along with the primary CompleteEASE features that are discussed.

## Section 4.1 Metal Substrates

| FEATURES IN THIS EXAMPLE |                         |
|--------------------------|-------------------------|
| • Save Optical Constants | Save Model              |
| • Building a Model       | B-Spline Layer (basics) |

## Section 4.2 Self Assembled Monolayer on Au

| FEATURES IN THIS EXAMPLE |                                     |
|--------------------------|-------------------------------------|
| • Parameter Uniqueness   | • Fixing B-Spline Optical Constants |

## Section 4.3 Absorbing Thin Films (B-SPLINE)

| FEATURES IN THIS EXAMPLE |  |
|--------------------------|--|
| • B-SPLINE Layer         | • <a href="#">Wvl. Range Expansion Fit</a> |
| • Starting Mat =         | • Selecting a Graph/Fit Range              |
| • Saving a Model         | • Zoom All                                 |

## Section 4.4 Absorbing Thin Films (Gen-Osc)

| FEATURES IN THIS EXAMPLE |                      |
|--------------------------|----------------------|
| • Gen-Osc Layer          | • Parameterize Layer |
| • Tauc-Lorentz           | • Cody-Lorentz       |

#### Section 4.5 Multiple Layer Film Stacks

##### NEW FEATURES IN THIS EXAMPLE

- |                     |   |
|---------------------|---|
| • Modifying a Model | • Global Fit/Pre-Fit with multiple layers |
|---------------------|---|

#### Section 4.6 Multiple Data Types (SE + T)

##### NEW FEATURES IN THIS EXAMPLE

- |                               |   |
|-------------------------------|---|
| • Appending Data              | • Fitting SE and Transmission data simultaneously |
| • <b>Parameter Uniqueness</b> | • Graph ScratchPad                                |

## 4.1. Metal Substrates

| FEATURES IN THIS EXAMPLE |                         |
|--------------------------|-------------------------|
| • Save Optical Constants | Save Model              |
| • Building a Model       | B-Spline Layer (basics) |

Substrate optical constants are an important consideration when modeling thin films. Although certain materials, such as crystalline silicon are well understood and will remain constant, others substrates such as glass and metals are more variable. In these cases, it is best to measure a bare substrate to determine optical constants. Glass substrates were considered in Section 3.4. We will consider a metal substrate for this example. Although the substrate is called a metal, it is actually a glass or silicon substrate that is coated with an optically opaque metal film. The measurement beam will not penetrate through the metal film, so we can consider it a substrate.

Open the “Au\_Substrate” data file. Substrates offer a special case, as the measurement involves only a single-interface (reflection from surface). The experimental measurement of Psi and Delta can be directly inverted to determine  $n,k$  using the pseudo-substrate approximation. To keep the optical functions smooth, a B-Spline layer can be used for the model. While this example will use the B-Spline, we will save the intimate details for a later example. In this exercise, we will build a model to fit any metal substrate and then save this model for future use.

To start, open the “Multilayer (empty)” model from the ADVANCED folder, and your screen should appear as in Figure 4-1. Left-click ( $\text{Ctrl}+\text{L}$ ) on the Substrate = “none”. This will bring up the “Open Material” dialog box. Choose the B-SPLINE material file from the Basic folder and press ‘Open’. Expand the B-Spline layer such that it can be edited.

- Set the resolution to 0.1eV.
- Set the Starting Mat = Ag (from the Metals location)

The resolution defines how closely spaced to apply “nodes” when allowing the optical constants to vary. The nodes are matched to the starting material file to provide an estimate before fitting. It is not necessary for the starting material to be the same as the material you have measured – this is the reason for choosing Ag in this example.

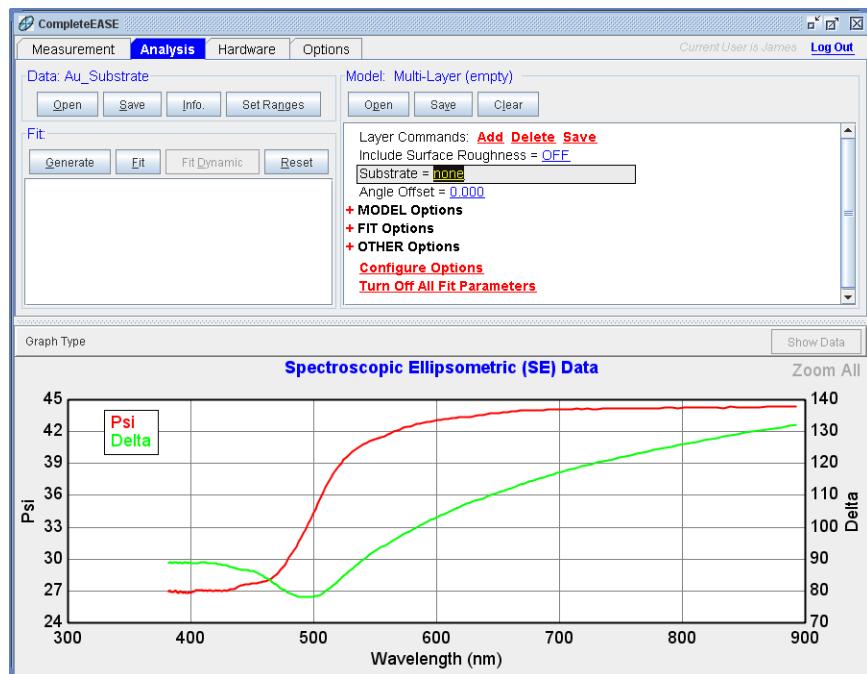


Figure 4-1. Starting the example for Au\_substrate with the Multi-Layer (empty) Model.

Generate data and then attempt the fit. It should quickly converge to the answer as shown in Figure 4-2.

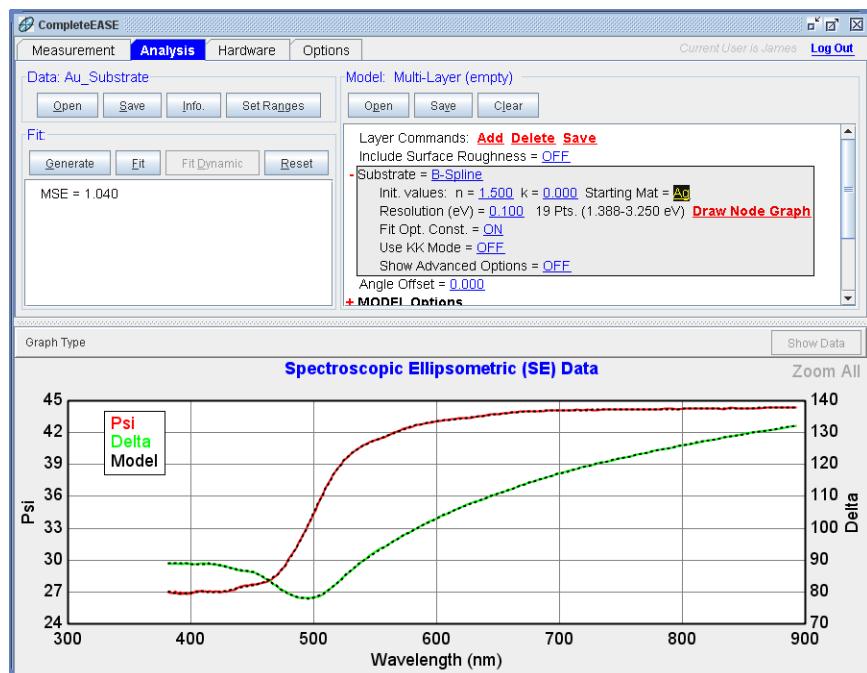


Figure 4-2. Fit to "Au\_Substrate" data using B-Spline layer.

To view the optical constants as shown in Figure 4-3, right-click on Substrate = “B-SPLINE” and choose “Graph Layer Optical Constants”. To view the spline points as in Figure 4-4, press on ‘Draw Node Graph’ within the B-Spline layer. The red and green curves are the smooth optical constants ( $e_1$  and  $e_2$ ) that are derived from the B-Spline fit, with the open circles showing the individual spline nodes.

As an exercise, change the Spline resolution to larger and smaller values and repeat the fit. Does the fit quality change?

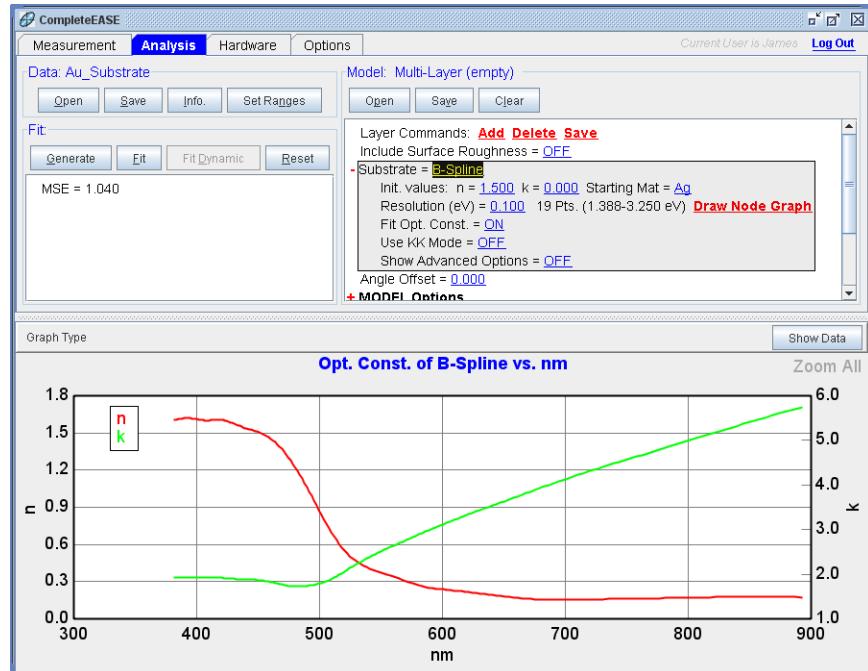


Figure 4-3. Resulting optical constants from B-Spline fit to “Au\_Substrate”.

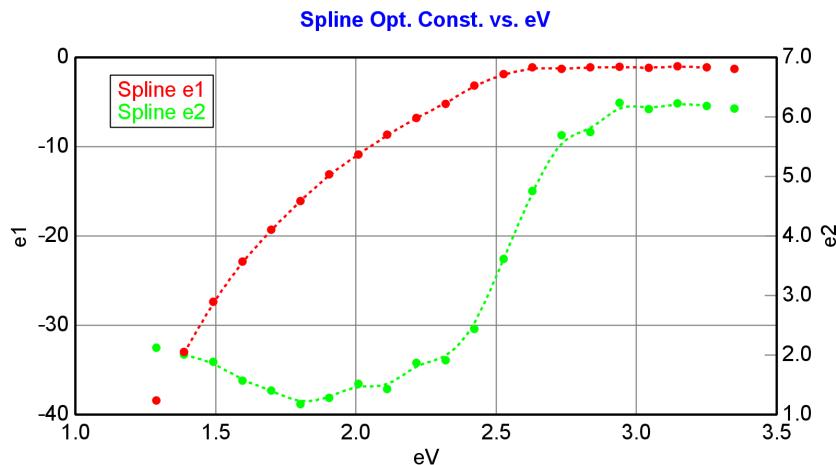


Figure 4-4. Spline points at 0.1eV resolution fit to the Au\_Substrate data.

## Save

When happy with results, press **Save** right above the model to save the gold optical constants. This opens the Save Layer Optical Constants dialog box as shown in Figure 4-5. Choose the “Tabulated” choice from the right. Next, press mouse on the substrate layer itself. After entering the file name and comment, the tabulated  $n,k$  at each measured wavelength will be saved for future use.

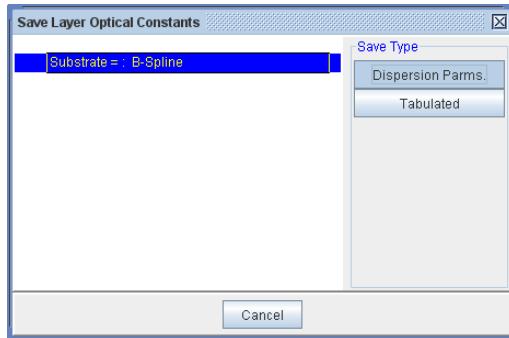


Figure 4-5. Save Layer Optical Constants dialog box.

## Save Layer Optical Constants

Alternatively, the layer optical constants can also be saved directly from a right-click menu over the Layer name (in this case “B-Spline”). This menu is shown in Figure 4-6. After pressing this selection, the user is asked whether to save the Parameterized optical constants (values used by equation to reconstruct the optical constants) or to save a tabulated list of optical constants at each measured wavelength.

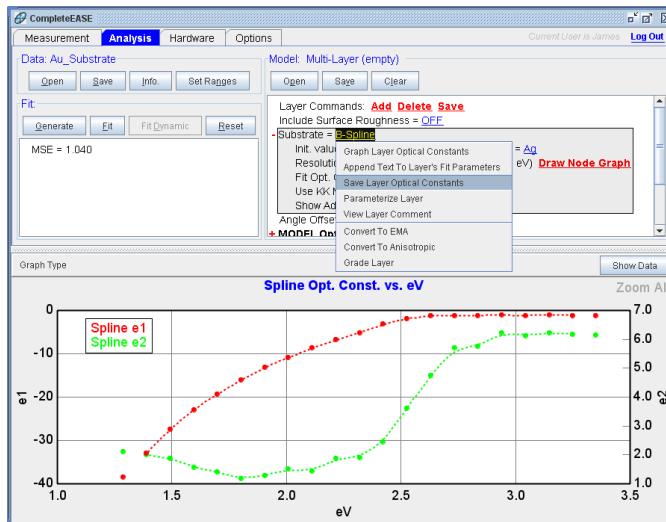


Figure 4-6. Right-click over a layer name to choose “Save Layer Optical Constants” from a drop-down menu.

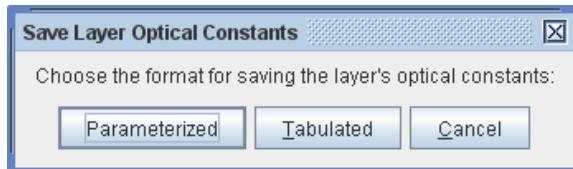


Figure 4-7. Choose whether to save the Parameterized optical constants (values used by equation) or a tabulated list of optical constants at each wavelength.

## Au Substrate Model

After optimizing the analysis for a new sample, the model can be saved for future use. Let's use this Au substrate as an example. If additional Au substrates will be measured in the future, a customized model would help reduce analysis time. For this example, modify two additional settings:

- Replace the “Ag” reference in the B-SPLINE layer with the metal optical constants saved in this example (previous step).
- Include Derived Parameters for both ‘n’ and ‘k’ of the substrate (make sure to change layer # to “0”).

Press the ‘Save’ button at the top of **Model**: pane to save the final model as “metal substrate example” as in Figure 4-8.

**NOTE:** If a model uses a new material file, both model and all material files must be located in the same folder.

Layer Commands: [Add](#) [Delete](#) [Save](#)  
 Include Surface Roughness = [OFF](#)

- Substrate = [B-Spline](#)

- Init. values: n = [1.500](#) k = [0.000](#) Starting Mat = [au\\_test](#)
- Resolution (eV) = [0.100](#) 19 Pts. (1.388-3.250 eV) [Draw Node Graph](#)
- Fit Opt. Const. = [ON](#)
- Use KK Mode = [OFF](#)
- Show Advanced Options = [OFF](#)

Angle Offset = [0.000](#)

+ MODEL Options

- FIT Options

- Perform Thickness Pre-Fit = [OFF](#)
- Use Global Fit = [OFF](#)
- Fit Weight = [N.C.S](#)
- Limit Wvl. for Fit = [OFF](#)
- Include Derived Parameters = [ON](#)

[Add Derived Parameter](#)

1: Type = [n](#) Layer # = [0](#) Wavelength = [632.8 nm](#) Name = [n\\_of\\_B-Spline @ 632.8 nm](#)  
 Low Spec. = [0.000](#) High Spec. = [0.000](#)

2: Type = [k](#) Layer # = [0](#) Wavelength = [632.8 nm](#) Name = [k\\_of\\_B-Spline @ 632.8 nm](#)  
 Low Spec. = [0.000](#) High Spec. = [0.000](#)

+ OTHER Options

[Configure Options](#)

[Turn Off All Fit Parameters](#)

Figure 4-8. Au Substrate model saved for future use.

## 4.2. Self Assembled Monolayer on Au

### FEATURES IN THIS EXAMPLE

- Parameter Uniqueness
- Fixing B-Spline Optical Constants

This example uses the Au substrate result from Section 4.1. Thus, you will need to complete 4.1 before proceeding to this example. To insure that the Au substrate model works before proceeding, open the “Au\_substrate” data file again and press fit. If the fit does not work, then repeat Section 4.1 before proceeding.

### Self-Assembled Monolayers

Self-Assembled Monolayers (SAMs) are very thin organic layers that consist of a single monolayer. Thus, they are generally less than 10nm thick and often closer to 1-2nm. Spectroscopic Ellipsometry is very sensitive to layers of this thickness, due to the phase information available from the measured Delta parameter. However, the index of refraction from such thin layers is not typically attainable. Instead, the nominal index of refraction must be assumed in order to fit the thickness. As layers become thicker than 10-20nm, spectroscopic ellipsometry gains sensitivity to index of refraction in addition to thickness. A common method for thinner layers is to measure a similar material as a thicker film. From the thicker film, the index can be measured and then fixed when measuring thinner layers. Because this approximation may not always be true for such thin layers, the measurement of SAMs is often qualitative and best used for comparison between multiple samples.

Open the “Organic on Au” data file and press ‘Generate’. The graph should appear as in Figure 4-9. The Model dashed curves will represent a bare Au surface, as they come from our model with only Au. Notice a shift in Delta toward lower values (at all wavelengths). This indicates the presence of a thin surface coating. A larger shift indicates a thicker film on the Au surface.

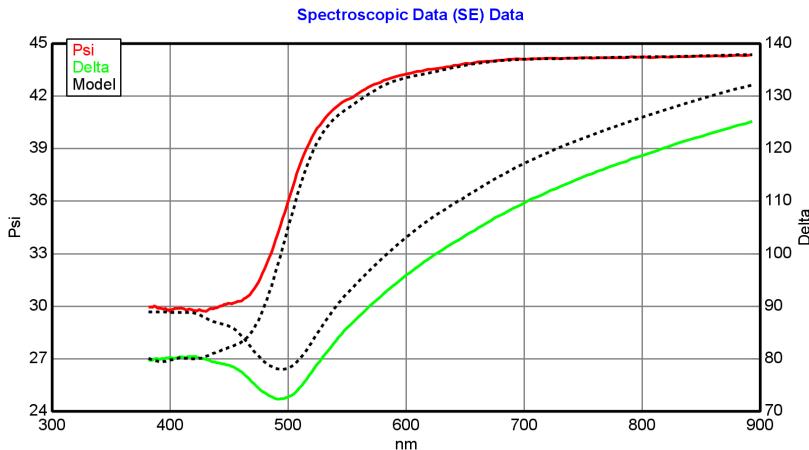


Figure 4-9. Data from “Organic on Au” compared to Generated Data from the bare Au surface. Notice the shift in Delta toward lower values for the coated sample, which indicates a surface coating.

Add a new layer to the Model by pressing **Model:>Add**. Position the blue bar above the Au substrate and click to add the layer. Choose Cauchy layer from the Basic folder and press ‘Open’. The default values for Cauchy layer will be close to the values needed for generic organic films. Thus, we will fix the optical constants for the Cauchy layer and only turn on the thickness as a fit parameter.

**BEFORE** proceeding, it is important to **FIX** the Au optical constants. If we fit at this time, the Au optical constants would also move and confuse our overall result.

To prevent the Au substrate optical constants from fitting, make sure to do the following:

- Turn OFF the “Fit Opt. Const.” command inside the B-Spline layer, as shown in Figure 4-10.
- Make sure the Global Fit is turned off.



Figure 4-10. Turn OFF the “Fit Opt. Const.” to insure the Au optical constants stay fixed at the values fit from the bare substrate data.

Turn on the Thickness of the Cauchy layer as a fit parameter (by clicking it with the right mouse button). Press ‘Fit’ and the resulting thickness of 7.48nm should be reported. If you get a different thickness, make sure the Au optical constants did not adjust from the previous fit.

## Parameter Uniqueness

We will use this result to demonstrate a feature in CompleteEASE that helps to visualize the model uniqueness. Go to the bottom of the **Model:** Panel and expand the **-OTHER Options**. In this section, press the **Parameter Uniqueness** command. You will be asked which of the fit parameters you want to select for testing. In this case, we have only fit the thickness, so choose Thickness #1, as shown in Figure 4-11.

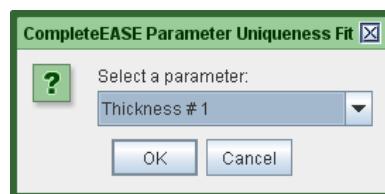


Figure 4-11. Choose fit parameter to test for Uniqueness.

Next, you need to enter the “Minimum value”, “Maximum value”, and “# of fit points”. These will define the test conditions. The parameter space between the

minimum and maximum will be divided into equal spacing to match the total number of points entered. Then, the fit will proceed with the test parameter (Thickness #1 in this case) fixed at each individual value. The MSE is captured from each fit for graphing.

For this example, choose a Minimum Value of 2.5nm, Maximum Value of 15nm, and 100 total points, as shown in Figure 4-12. You will get a warning that no other fit parameters are selected, as shown in Figure 4-13. This is okay, as the test will still proceed to show the MSE profile as the Cauchy thickness is varied, as shown in Figure 4-14.

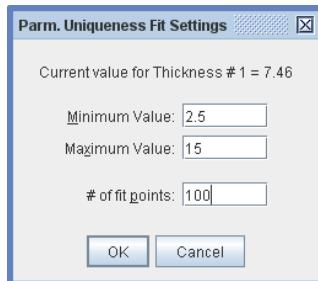


Figure 4-12. Settings for Parameter Uniqueness Test.



Figure 4-13. Warning message shown when the only fit parameter turned on is the test parameter. It is okay to proceed past this warning to see the MSE profile as that single fit parameter is varied.

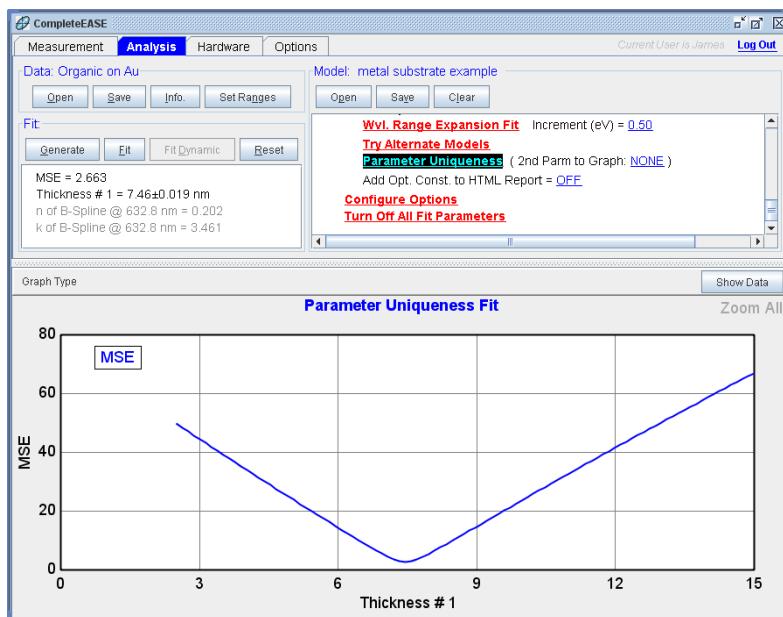


Figure 4-14. MSE profile from Uniqueness test of the thickness for thin Self-Assembled monolayer on Au when the optical constants are fixed.

Right-click on the graph area and copy the MSE profile data to the Graph ScratchPad. This will allow us to compare the MSE curve for this fit with our next test.

Next, allow the A, B, and C parameters in the Cauchy layer to fit. Repeat the Parameter Uniqueness test with the same settings for Thickness #1. This time, the result should appear as seen in Figure 4-15. Add this result to the Graph ScratchPad and then view the ScratchPad to allow comparison of the two tests as shown in Figure 4-16.

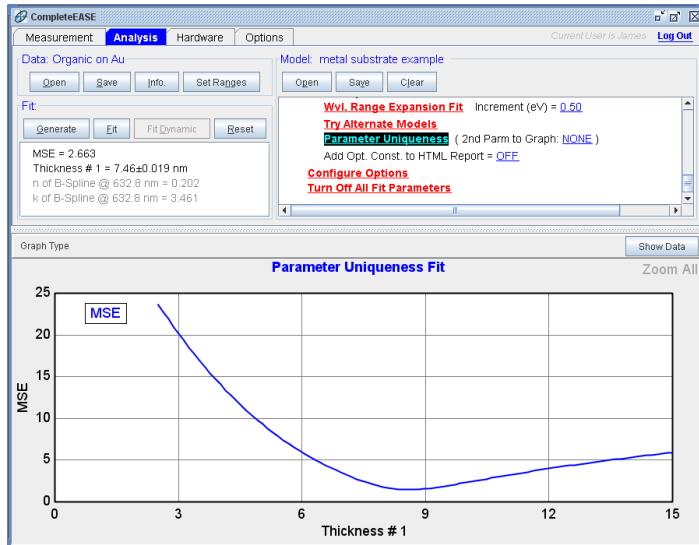


Figure 4-15. MSE profile from Uniqueness test of the thickness when the Cauchy parameters for thin layer are allowed to vary at each point.

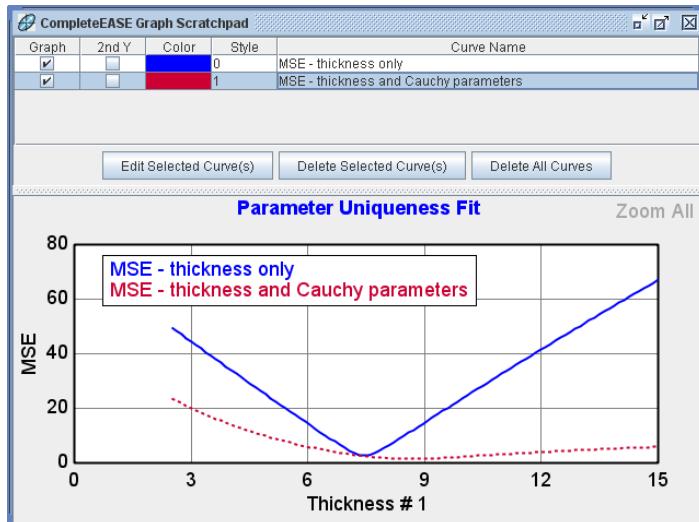


Figure 4-16. Comparison of MSE profiles from both tests, as seen in the Graph ScratchPad.

## 4.3. Absorbing Thin Films (B-SPLINE)

| FEATURES IN THIS EXAMPLE                                 |  |
|--|--|
| • B-SPLINE Layer<br>• Starting Mat =<br>• Saving a Model | • <a href="#">Wvl Range Expansion Fit</a><br>• Selecting a Graph/Fit Range<br>• Zoom All |

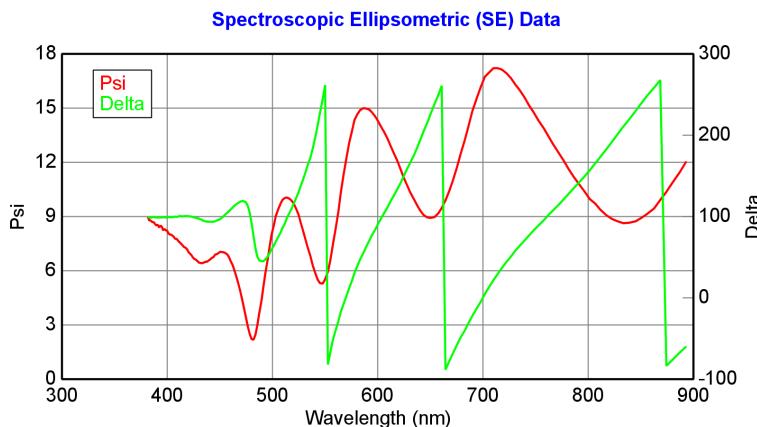
SE measurements on absorbing films are more difficult to analyze compared to transparent films. This is because the general structure of the film optical constants ( $n, k$ ) versus wavelength is not always known before the measurement. To handle absorbing film analysis problems, CompleteEASE implements a couple special layer types: a “B-Spline” layer which allows arbitrary flexibility in  $n, k$  versus wavelength, and the “Gen-Osc” layer which uses a summation of standard oscillator lineshapes. The B-Spline is described in this example, while the Gen-Osc will be described in the next example.

The B-Spline layer is perfect for materials that are partially transparent and partially absorbing – such that the ellipsometer witnesses the onset of absorption. A few example materials of this nature include:

- A-SI, A-GE, A-SIGE
- ZnS, ZnSe
- Most organics, such as polyimide, PEDOT, P2VP, Alq3, P3HT, photoresists, and many more.
- Diamond-like carbon (DLC)
- SIC
- TiO<sub>2</sub>

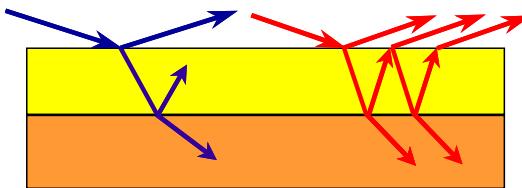
### Identifying an Absorbing Film

Open the “SiC on Si” data file from the EXAMPLES folder. Notice that Psi and Delta oscillate (Figure 4-17) as we have seen for transparent film examples. These oscillations are caused by interference between light that reflects from the film surface and light that travels through the film and returns from the bottom interface. The thicker the film is, the more oscillations that will appear.



*Figure 4-17. Data from SiC film on Silicon. The interference oscillations in data suggest the film is transparent at longer wavelengths, while the decrease in amplitude of these oscillations at short wavelengths indicates UV absorption.*

Unlike the transparent films we have witnessed, the interference oscillations decrease in amplitude toward shorter wavelengths. This is a strong indication of absorption in the ultraviolet spectrum. The oscillations are damped, as less light is able to penetrate the film and return to the surface to interfere with the top-reflected light. This concept is illustrated in Figure 4-18. To model the SiC film on Silicon will require a material file that can describe both transparent and absorbing regions.



*Figure 4-18. Interference oscillations occur when the light can travel through a thin film and return from the bottom interface (red). If the light is absorbed, the light only comes from the top-surface (blue) and will not produce interference.*

## Si with Absorbing Film

Now, open the “Si with Absorbing Film” model from the BASIC folder and click ‘Fit’. The results should appear as shown in Figure 4-19. To view the optical constants of the film, right-click ( $\text{F} \text{R}$ ) on the “B-Spline” layer in the model and select “Graph Layer Optical Constants”. The resulting optical constants (which are the optical constants for the SiC film) are shown in Figure 4-20. The film is essentially transparent ( $k \sim 0$ ) at longer wavelengths ( $\lambda > 600\text{nm}$ ) with a gradual increase in absorption at shorter wavelengths. The film index ( $n$ -red curve) also increases toward shorter wavelengths.

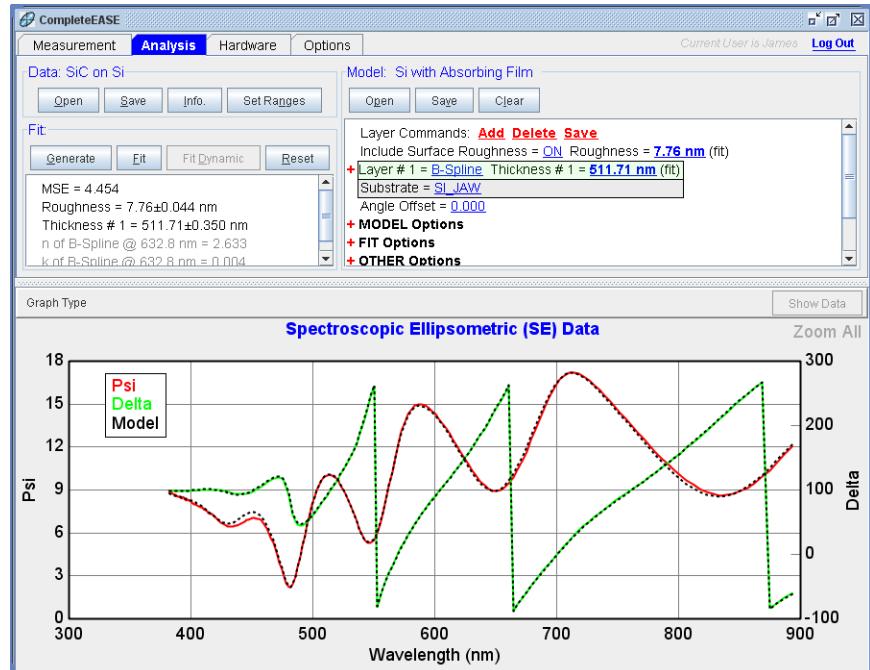


Figure 4-19. Data fit to SiC on Si using the Si with Absorbing Film model.

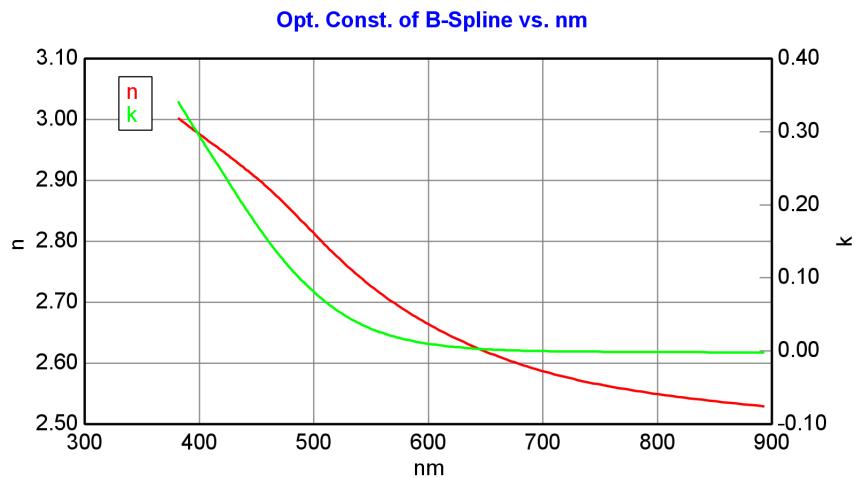


Figure 4-20. Optical constants for SiC film using the "B-Spline" layer.

## The “B-Spline” Layer

The “Si with Absorbing Film” model settings are shown in Figure 4-21; the “+” next to “Layer #1” was clicked to expand the “B-Spline” layer. The B-Spline layer specifies the optical constants versus wavelength using a series of control points which are equally spaced in photon energy (eV). The approximate spacing of the control points is controlled by the “Resolution (eV) =” field and the resulting number of control points within the current spectral range is listed after this value. Basis spline curves (which are by definition smooth and continuous in the 0th, 1st, and 2nd derivatives) are used to interpolate the optical constants between the control points.

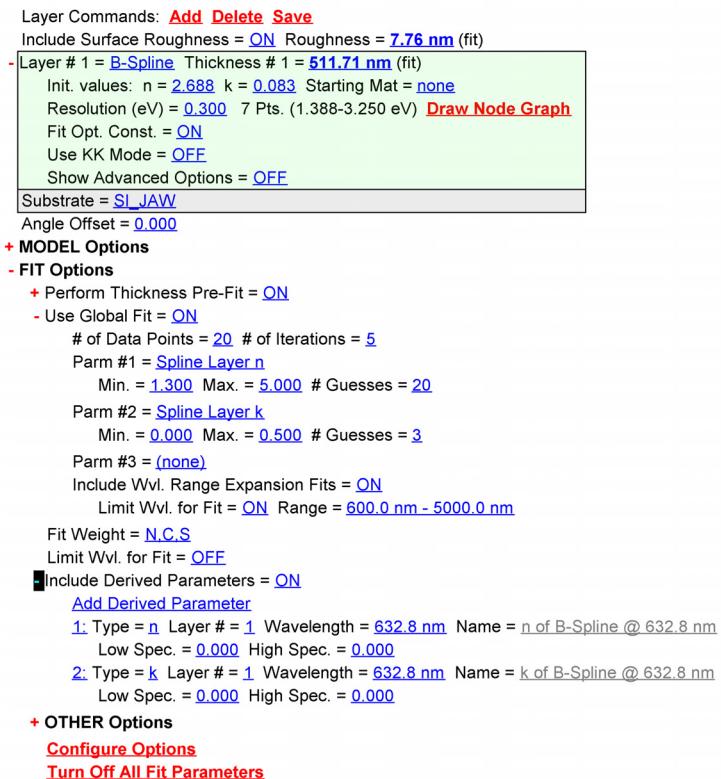


Figure 4-21. Settings for the “Si with Absorbing Film” optical model.

Clicking on “Draw Node Graph” displays the graph shown in Figure 4-22. This graph shows the location of the spline control points. The B-Spline layer always works in terms of the complex dielectric function  $\epsilon = \epsilon_1 + i\epsilon_2 = (n + ik)^2$ , which is often written as “e1 & e2”. One set of control points (and associated spline curve) is used to specify the dispersion in “e1” and a second set of control points is used to describe “e2”. Using a smaller “Resolution” value adds more control points, resulting in more flexibility to accommodate sharper features in the dielectric constant spectra. However, setting the Resolution too low can result in unwanted noise or unphysical artifacts in the dielectric function spectra.

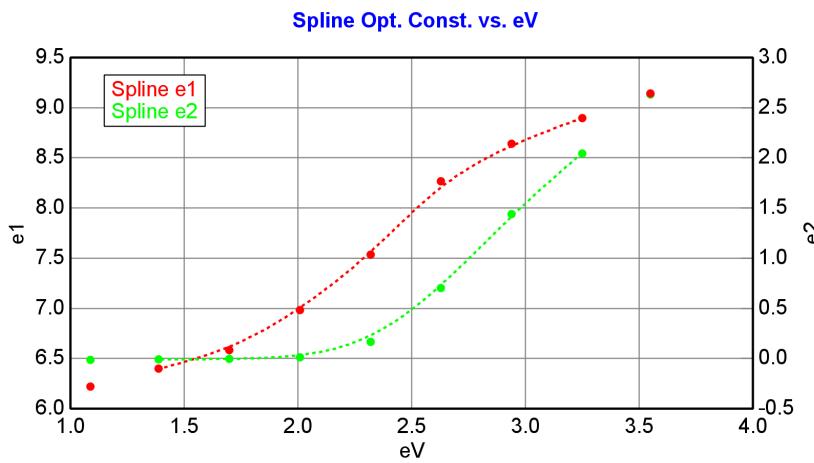


Figure 4-22. B-Spline dielectric function “e1 & e2”, showing the location of the “control points” (red and green dots), which are equally spaced in eV.

There are two ways to initialize the B-Spline layer control point values:

1. Click on the “n =” and/or “k =” fields which sets all control points to this new value over the entire spectral range.
2. Click on “Starting Mat =” which chooses control points to match the optical constant values from the specified material file.

The “Si with Absorbing Film” model uses the first method combined with the “Global Fit” option to search a range of  $n$  and  $k$  values for the film. The “Use Global Fit” section in Figure 4-21, specifies twenty  $n$  values ranging from 1.3 – 5 and three  $k$  values ranging from 0 – 0.5.

Note: The Global Fit is a slow procedure and should be turned off if you have a good starting guess for the optical constants. In this manner, you can save significant time by avoiding the “automated” recipe – especially when dealing with multi-angle data sets.

The “Fit Opt. Const.” button allows the user to turn on and off the fitting of spline points from within the B-Spline. Thus, an absorbing material could be fit using the B-Spline and then the “Fit Opt. Const.” button can be toggled to OFF to fix the optical constants of this layer in place for further analysis.

Note: To FIX optical constants, the Global Fit also needs to be turned off

In the B-Spline layer, the “Use KK mode” is an advanced calculation that maintains Kramers-Kronig consistency between the resulting e1 and e2 spline curves. When this feature is ON, the optical constants will be constrained to a physical shape – thus it should provide further assurance that the resulting optical constants are correct. This feature will also reduce the total number of fit parameters, as only the e2 spectra is described with a series of spline points while the e1 spectra is calculated via the Kramers-Kronig transformation. Additional “Advanced Options” in the B-Spline layer are further documented in Section 8.6.

## Wavelength Range Expansion (WVL-EXPAND) Fit

The “Si with Absorbing Film” model uses a Wavelength Range Expansion (WVL-EXPAND) fit within the Global Fit. This is explained in the subsequent section. First, let’s demonstrate how the WVL-EXPAND fit routine works. The principle behind the WVL-EXPAND fit is that a model may work better over a narrower selection of wavelengths as compared to the entire measured range. Organic films are an excellent example as they are typically transparent at longer wavelengths with absorption only in the UV. Thus, a Cauchy is often adequate for longer wavelengths but is not applicable to shorter wavelengths when the film becomes absorbing. The B-SPLINE layer can work in both transparent and absorbing regions, but may find the correct starting solution more readily in the transparent region. The transparent region minimizes the fit complexity as only the index needs to be determined.

### Range-Selecting Wavelengths

To manually perform a WVL-EXPAND fit, we first need to learn how to select a subset of data over a specific wavelength range. This is simple in the CompleteEASE program. First, choose a wavelength that will serve as an end-point for the new data subset. Left-click ( $\text{Ctrl} + \text{L}$ ) the mouse on this wavelength and hold the mouse button down while dragging to the opposite end-point wavelength. If the mouse drags off the side of a graph, all wavelengths in that direction will be included (even expanding the graph to include wavelengths not shown).

As an exercise, open any data file and try the following:

1. Range-select 600-700nm using the mouse (Figure 4-23).

*As you drag the mouse across the graph with the left-button held down, it should create a “black area” on the graph to show the range of wavelengths selected.*

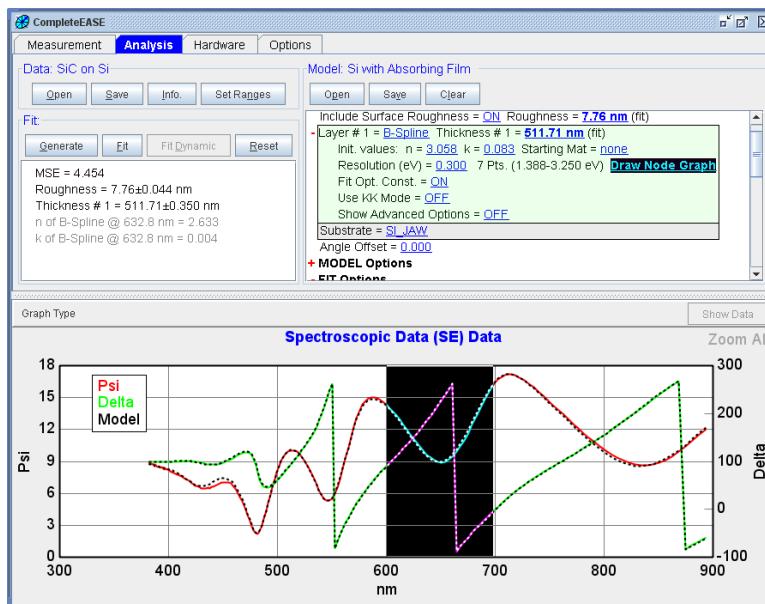


Figure 4-23. Range-selecting wavelengths between 600 and 700nm.

2. Range select wavelengths of 600nm and above. For this, start the mouse-button just inside the current graph (near 600nm) and then drag beyond the right graph boundary to incorporate all longer wavelengths (Figure 4-24).

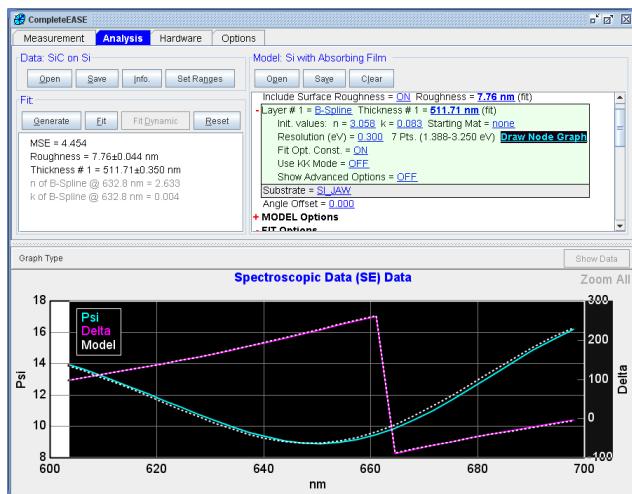


Figure 4-24. Expanding the current wavelength range to longer region.

- Finally, select the entire wavelength range. This is accomplished by dragging the mouse over both graph boundaries or pressing ‘Zoom All’ at the top-right of the graph pane (Figure 4-25).

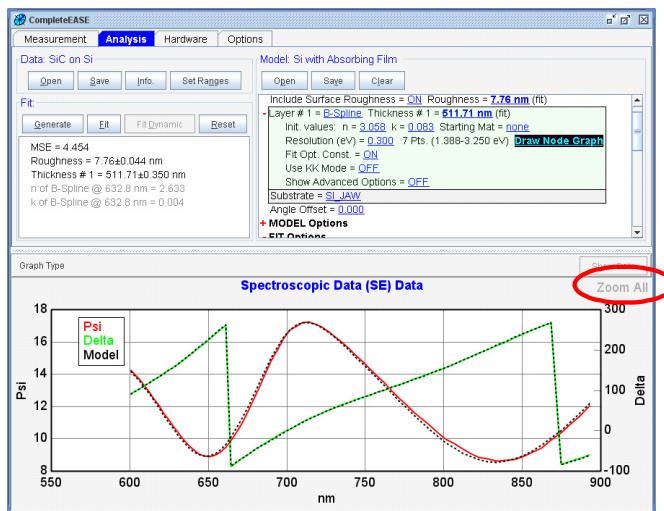


Figure 4-25. Press ‘Zoom All’ to select the entire wavelength range.

Now, let’s return our attention to the WVL EXPAND fit. This fit works by taking a limited wavelength range (as selected by the user), applying the current fit, and then gradually increasing the range to both shorter and longer wavelengths until the entire data set is included in the fit. The fit is performed at each new increment of wavelengths.

To manually perform a WVL EXPAND fit, you choose the desired starting wavelength region, and press **+OTHER Options>WVL. Range Expansion Fit** at the bottom of the Model pane.

## **WVL-EXPAND Fit with B-SPLINE Layer**

The B-SPLINE layer works very well with the WVL-EXPAND fit. As the wavelength range is expanded, the number of spline control-points automatically increases to match the new wavelength range. The additional points are initialized by extrapolation of the existing model, but then are fit to match the experimental measurement. The true power of the WVL-EXPAND fit can be seen by extending this fit to include Global Fitting (as described in next section).

## **Global Fits with WVL-EXPAND Fitting**

The WVL-EXPAND fit can also be used in conjunction with the Global Fit. When this option is “ON”, a WVL-EXPAND fit is performed at every trial of the global fit. Thus, each fit will begin over a restricted range of wavelengths, followed by an expansion of wavelengths to the entire range. The MSE of the final expanded fit is compared between all trial fits to determine which result gives the best agreement. The best fit from all the Global Guesses is reported.

### **- FIT Options**

- + Perform Thickness Pre-Fit = ON**
- Use Global Fit = ON**
  - # of Data Points = 20 # of Iterations = 5
  - Parm #1 = Spline Layer n
    - Min. = 1.300 Max. = 5.000 # Guesses = 20
  - Parm #2 = Spline Layer k
    - Min. = 0.000 Max. = 0.500 # Guesses = 3
  - Parm #3 = (none)
  - Include Wvl. Range Expansion Fits = ON
    - Limit Wvl. for Fit = ON Range = 600.0 nm - 5000.0 nm
    - Fit Weight = N.C.S
    - Limit Wvl. for Fit = OFF
  - + Include Derived Parameters = ON**

*Figure 4-26. Global Fit and Wavelength Range Expansion Fit regions of the model for absorbing film using B-Spline layer.*

Figure 4-26 shows the additional options available when a WVL-EXPAND fit is turned “ON”:

### ***Limit Wvl Range for Fit***

This first option chooses whether to start with the user-selected wavelength range (OFF) or the wavelength range chose within the model (ON). Typically, this option would be turned ON for automatic models, as it does not require the user to decide where to start. However, it can be turned OFF when first testing a model to determine how to setup the initial wavelength range.

### ***Wvl. Expansion Wvl. Range***

When the “Limit Wvl. Range for Fit” option is turned “ON”, this selection dictates the starting wavelength range for the WVL-EXPAND fit. This option is helpful when automating a model.

The Global fit with WVL-EXPAND fit is a very powerful data analysis algorithm which “automatically” works for a wide range of samples. Here are some hints for “tuning” the algorithm to analyze data sets when the default values fail:

- Adjust the “Spline Layer n” and “Spline Layer k” ranges to values which closely bracket the nominal optical constants.
- For thicker films (i.e., data sets with many oscillations) it may be necessary to increase the “# Guesses”; thinner films can use fewer “# Guesses”, which will reduce the data analysis time.
- For thin films (<100 nm) the WVL-EXPAND Fit may not be required.
- For very thick films (>1 – 2 microns), it may be necessary to specify a more limited spectral range (it is preferable that the film is transparent in the limited spectral range).
- Unless the nominal layer thickness is accurately known (and set in model), “Perform Thickness Pre-Fit” option should be ON.
- Before beginning the global fit, make sure all other model parameter values are set appropriately (for example, if Surface Roughness is included in the fit, its starting value should probably be zero).

## 4.4. Absorbing Thin Films (Gen-Osc)

| FEATURES IN THIS EXAMPLE |                      |
|--------------------------|----------------------|
| • Gen-Osc Layer          | • Parameterize Layer |
| • Tauc-Lorentz           | • Cody-Lorentz       |

In the previous example, we introduced the analysis of absorbing thin films via the B-Spline layer. Another method for absorbing films that can be used independently or after initial B-Spline modeling is the Gen-Osc layer. The Gen-Osc models the absorbing features by describing the shape of the absorption. This example demonstrates the common application of the Gen-Osc layer.

### Parameterize Layer

The resulting B-Spline optical constants from the “Si with Absorbing Film” model fit may be completely adequate for many applications. While the B-Spline layer guarantees the optical constants versus wavelength will be “smooth”, it does not always guarantee they are physical (that is, Kramers-Kronig consistent). Furthermore, the B-Spline layer requires many fit parameters (two times the number of control points), which may lead to correlation in the data fit. Once the general shape of the optical constants are determined using the B-Spline layer, it is often desirable to parameterize the optical constants with a simple analytic expression. The “Parameterize Layer” command can conveniently perform this procedure.

NOTE: The Goal of Layer Parameterization is to match the shape of  $n, k$  from the B-SPLINE fit using a dispersion model.

To parameterize the B-Spline optical constants for the SiC film in the previous example, right-click on the B-spline layer and choose “Parameterize Layer” from the drop-down menu, as shown in Figure 4-27. This opens “Parameterize Layer” dialog box as shown in Figure 4-28, with the B-Spline layer optical constants plotted in the graph. The default model (Gen-Osc) will automatically open in this window with a starting oscillator (in this case, Cody-Lorentz).

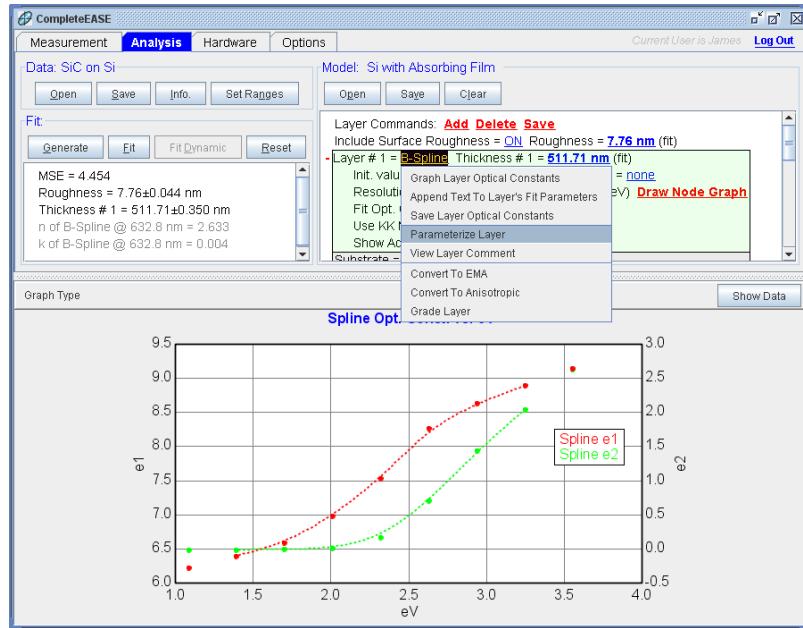


Figure 4-27. Right-click on a layer to drop-down menu, then press “Parameterize Layer”.

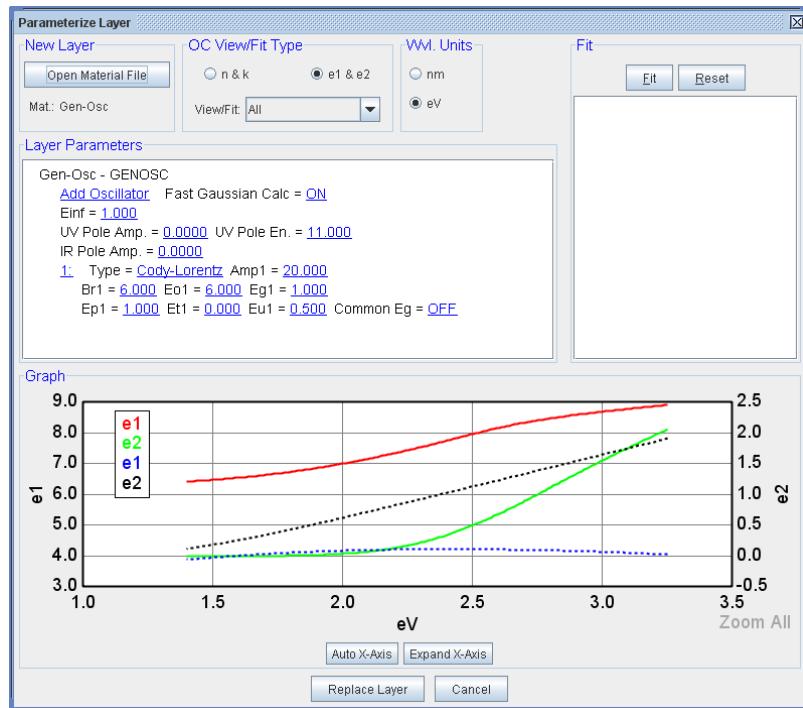


Figure 4-28. Parameterize Layer dialog box, showing starting optical constants of the layer along with the default Cody-Lorentz oscillator.

The “Gen-Osc” material file (which stands for General Oscillator) allows a combination of various oscillator lineshapes. We want to match the shape of SiC optical constants with an oscillator. There are many choices which are detailed in Section 8.6. For this example, left-click on the “Cody-Lorentz” name and choose “Tauc-Lorentz” from the Input box, as shown in Figure 4-29.

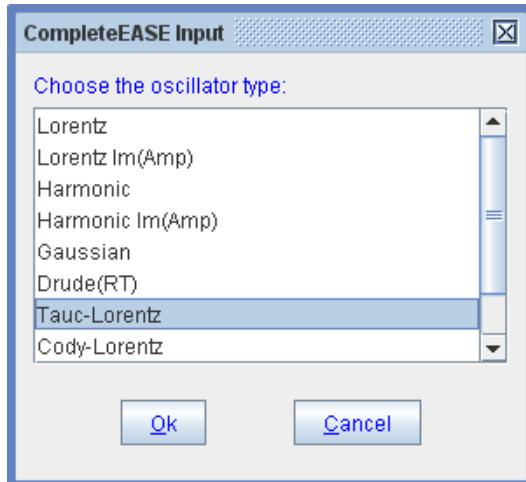


Figure 4-29. Input box with choices of different oscillator types.

The basic steps for matching optical constants with a new oscillator model are as follows:

1. Match e2 by adjusting and then fitting the oscillator parameters.
2. Match e1 by adjusting and then fitting the e1offset or Pole values.
3. Final adjustment to all parameter to fit both e1 and e2.

Each of these three steps will be demonstrated for the SiC example, where we match the SiC B-Spline results with the Tauc-Lorentz oscillator parameters.

### **Step 1: Match Imaginary Part.**

Most oscillators are Kramers-Kronig consistent. This provides an internal coupling between the real ( $e_1$ ,  $n$ ) and imaginary ( $e_2$ ,  $k$ ) optical properties. As we adjust the oscillator parameters to match the shape of  $e_2$  from our B-Spline result, we will in-turn be automatically adjusting the  $e_1$  shape via the KK transformation. Step 2 will allow us to adjust additional parameters that will only affect  $e_1$ , which is why it is important to start with the  $e_2$  matching.

The new Gen-Osc layer in CompleteEASE version 4+ has improved controls to move the oscillator  $e_2$  shape to match the reference values. To access these controls, LEFT-click your mouse on the number next to the Tauc-Lorentz oscillator, as shown in Figure 4-30. Note that the selected oscillator will now have a shaded box surrounding the number.

NOTE: It is important to LEFT-click the mouse on oscillators you wish to adjust as RIGHT-clicking will delete that oscillator from the list. If you do this accidentally, simply press the **Add Oscillator** line.

When an oscillator is selected, control boxes will appear to allow manipulation of the center energy, amplitude, broadening and possibly the bandgap. Not all of the gray squares will appear if the oscillator values are outside the graphed range. To view all of the control points, as shown in Figure 4-31, press the ‘Expand X-Axis’ button at the bottom of the dialog box.

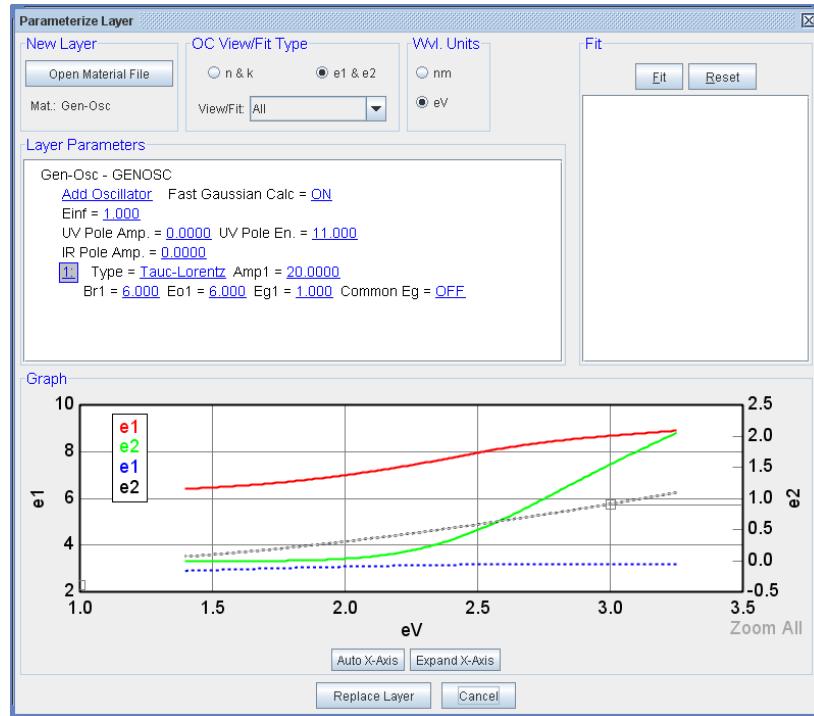


Figure 4-30. Left-clicking on the number next to an oscillator selects that oscillator for manipulation.

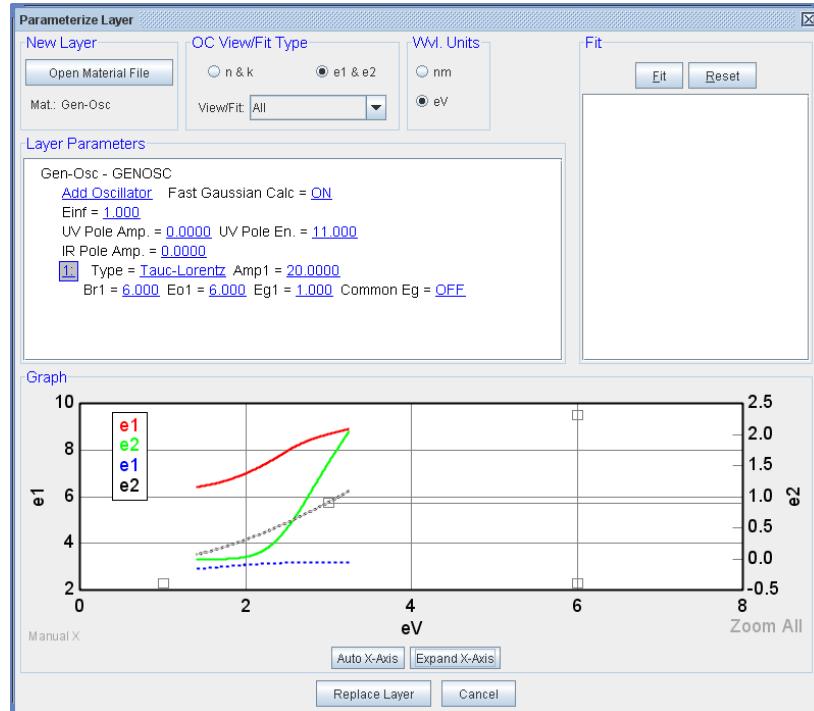


Figure 4-31. Press the 'Expand X-Axis' button to view all of the control points that manipulate the oscillator, even if they are outside the measured spectral range.

Before we adjust any of the control points, it is easier to visualize the oscillator if we change the **OC View/Fit Type** to “Imaginary Part Only”. This will show the green curve of e2 (or k) from our B-Spline fit along with the dashed gray curve from the oscillator we are adjusting. The goal is to match these two curves. If you position your mouse over any of the gray control boxes, your pointer should change to an XY arrow to show that you can now adjust that control box. This is shown in Figure 4-32, where the top control box is selected. This top control box can move both the amplitude and the center energy. Practice moving the different control boxes to better match the dashed curve to the green B-Spline data.

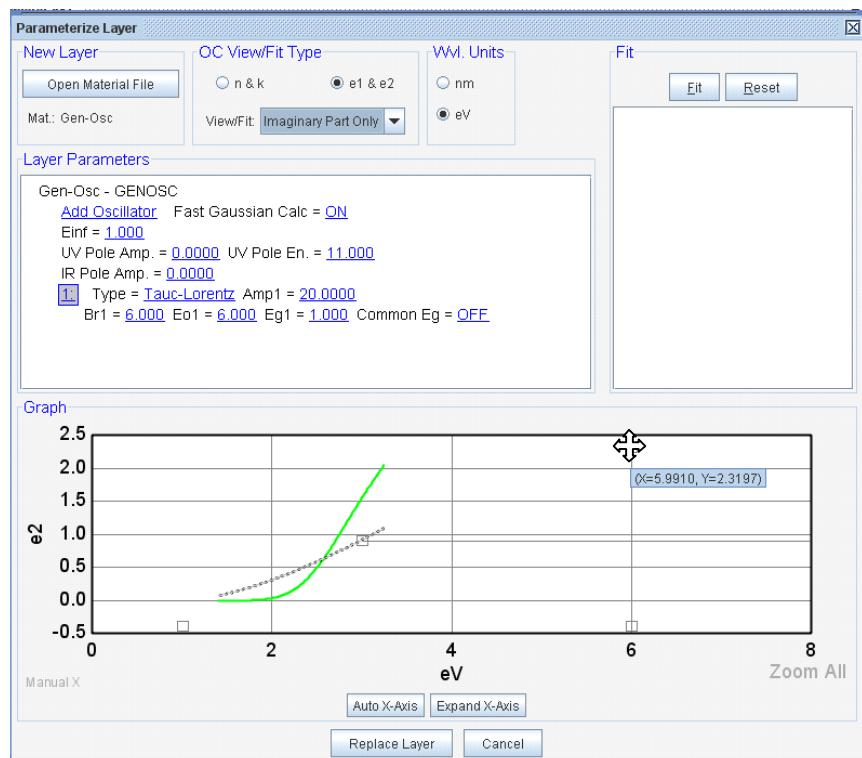


Figure 4-32. Cursor positioned above the top control point turns to an XY Arrow to show that this control point can be adjusted to change the shape of the selected oscillator.

After the oscillator parameters have been adjusted to better match the reference e2 shape, right-click ( $\text{Ctrl}+\text{R}$ ) on the “Amp.”, “Br”, “Eo”, and “Eg” parameters. This will turn them ON as fit parameters. Click the ‘Fit’ button. In this case, we are not fitting the experimental data, but rather matching the imaginary oscillator shape (via the parameters) to the reference optical constants.

The fit varies the oscillator parameters to match the imaginary curve shape as entered from the B-Spline. Figure 4-33 displays the fit results; the black dashed curve in the graph is calculated using the Tauc-Lorentz dispersion formula.

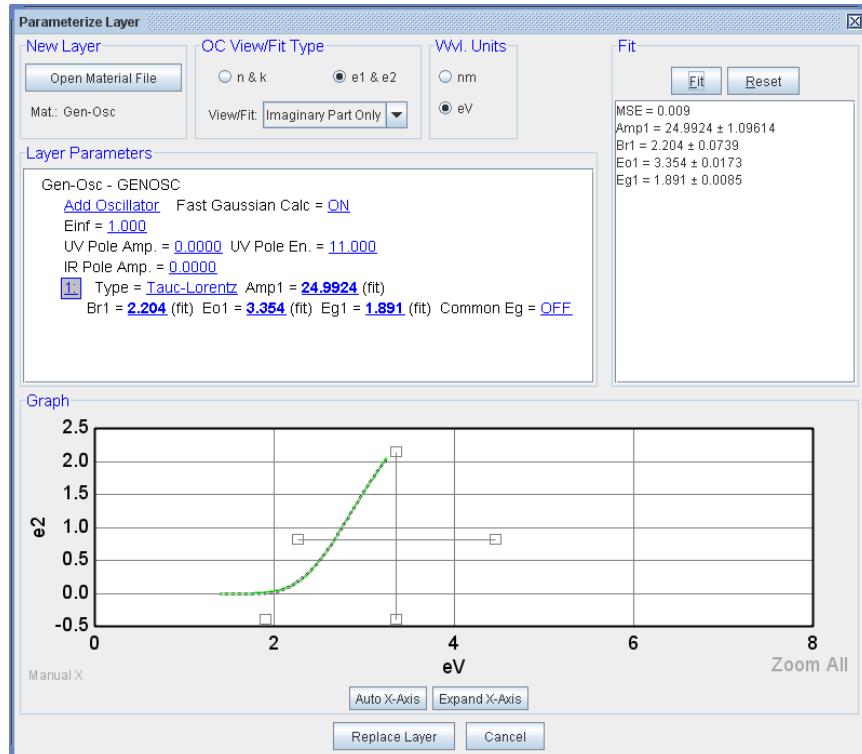


Figure 4-33. Fit to imaginary values of SiC using a single Tauc-Lorentz oscillator.

### Step 2: Match Real Part.

When finished matching the imaginary part with an oscillator, change the OC View/Fit Type to “Real Part Only”. The oscillator list will be hidden from view, as the only parameters allowed to vary during “Real Part Only” fitting are the Einf, and two Poles, as shown in Figure 4-34. Poles are unbroadened oscillators that are placed outside the measured spectral range to affect the real part of the optical constants in the same manner that a strong absorption in that spectrum would. Thus, the UV pole will pull the index up toward the short wavelengths while the NIR pole will pull the index down toward longer wavelengths. The Einf value adds a constant offset to all index values, which approximates the effects of absorptions that are significantly distant from the measured wavelengths.

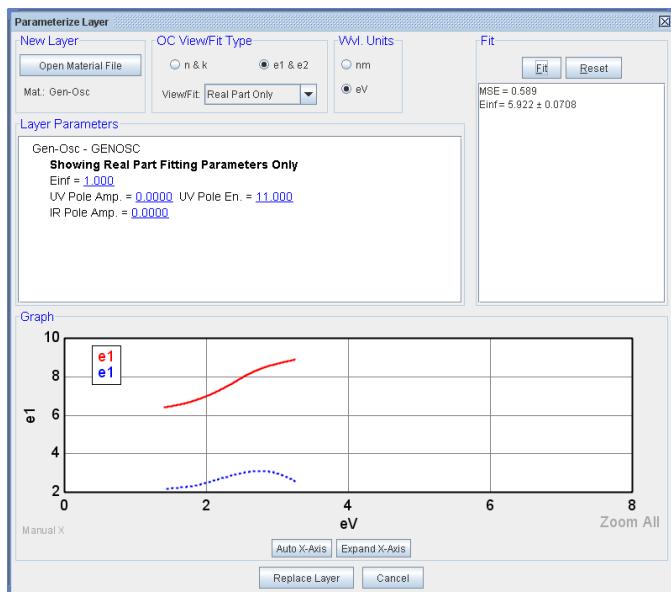


Figure 4-34. The only parameters required when fitting “Real Part Only” are the Einf, and two Poles.

For this example, it is best to adjust the parameter values before starting the fit. When values are changed in the **Layer Parameters** box, the optical constant graph is automatically updated. Enter a UV Pole Amplitude of 100 and the curve raises upward. The parameters can also be “dialed in” by positioning the mouse above a parameter, holding down the “Shift” key, and rolling the mouse wheel. Figure 4-35 shows the curves after the UV Pole Amplitude has been raised to get closer to the reference curve. However, the “tilt” of the curve does not match. This is because the UV Pole Position may also need to be adjusted. In general, the closer the UV Pole energy to the measurement range, the more “tilting” that will occur.

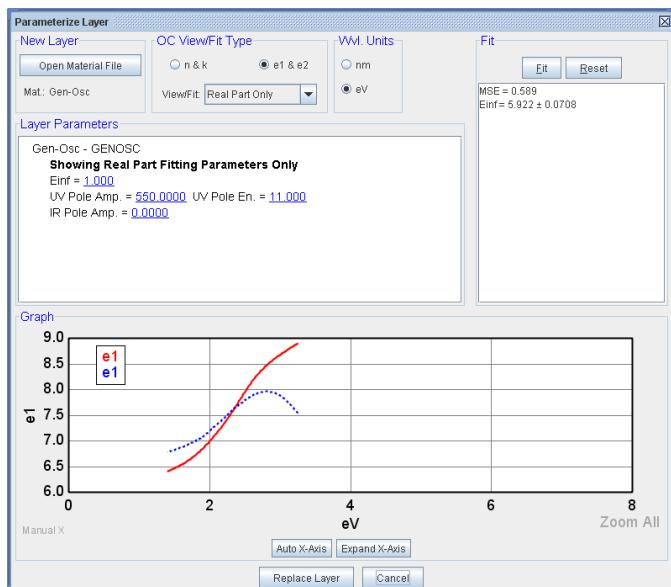


Figure 4-35. Increasing the UV Pole Amplitude also raises the Gen-Osc “e1” value, but the blue curve does not match the “tilt” of the red reference curve from our B-Spline. This will require adjustment of the UV Pole Energy.

After adjusting the UV Pole Position and Energy to better match the reference B-Spline curve, the two values are “fit” to give the best match. Afterward, the Einf value was also added to the fit to get a good match, as shown in Figure 4-36.

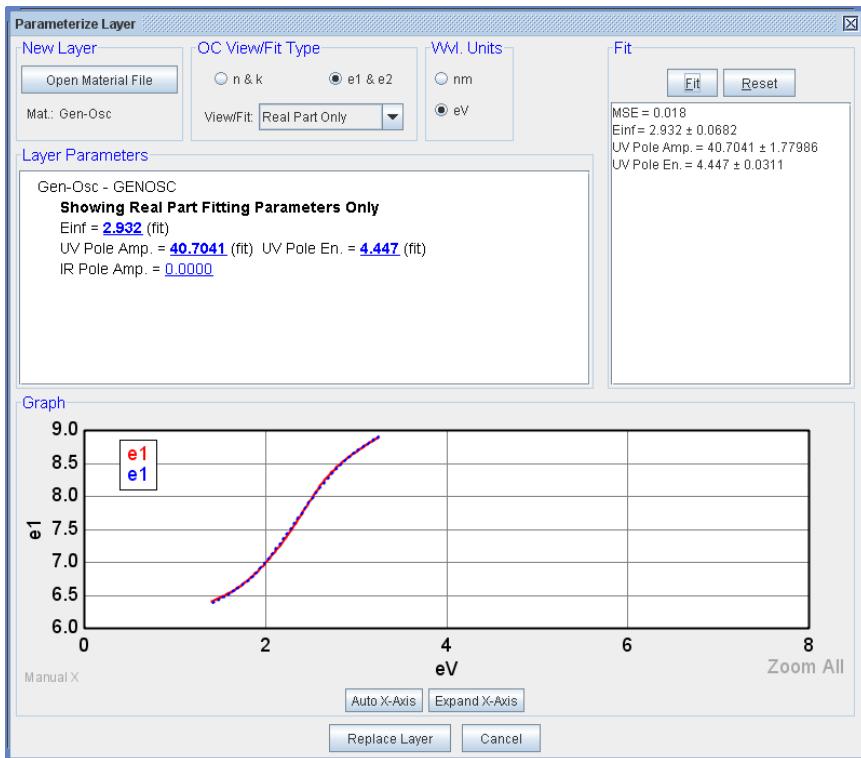


Figure 4-36. Fit to the B-Spline reference e1 value was achieved by varying (and fitting) the UV Pole Amplitude, Energy, and Einf.

### Step 3: Match All.

If Step #1 and #2 were successful, the Gen-Osc will not match both real and imaginary values of the reference. However, there can be some correlation between values used to match the e2 curve and those used to match the e1 curve. Thus, a final fit is often recommended with the **OC View/Fit Type** set to “All”. The most common correlation occurs when one of the oscillators is centered outside the measurement spectral range and thus can contribute in different ways to the e1 value (via KK transformation), as the amplitude and center energy can adjust and still provide a similar “tail” of absorption in the measured wavelength range.

## Replace Layer

After you are happy the Gen-Osc matches both real and imaginary components of the reference B-Spline, press ‘Replace Layer’ to apply the new oscillator model in place of the B-SPLINE layer, as seen in Figure 4-37. The new oscillator can now be used to fit data. Press ‘Fit’ to see how well the Tauc-Lorentz oscillator can describe the experimental data. If further samples with similar optical constants are measured, this model could be used directly – skipping the B-SPLINE layer step. If the parameterization is not successful, press ‘Cancel’ to revert to the existing layer optical constants.

Note: Fitting data is different than Fitting within the Parameterize Layer dialog box. In the former, you are allowing the oscillator parameters to adjust to best match the experimental SE data while the latter is used to get starting oscillator parameter values by fitting the shape of the reference optical constants.

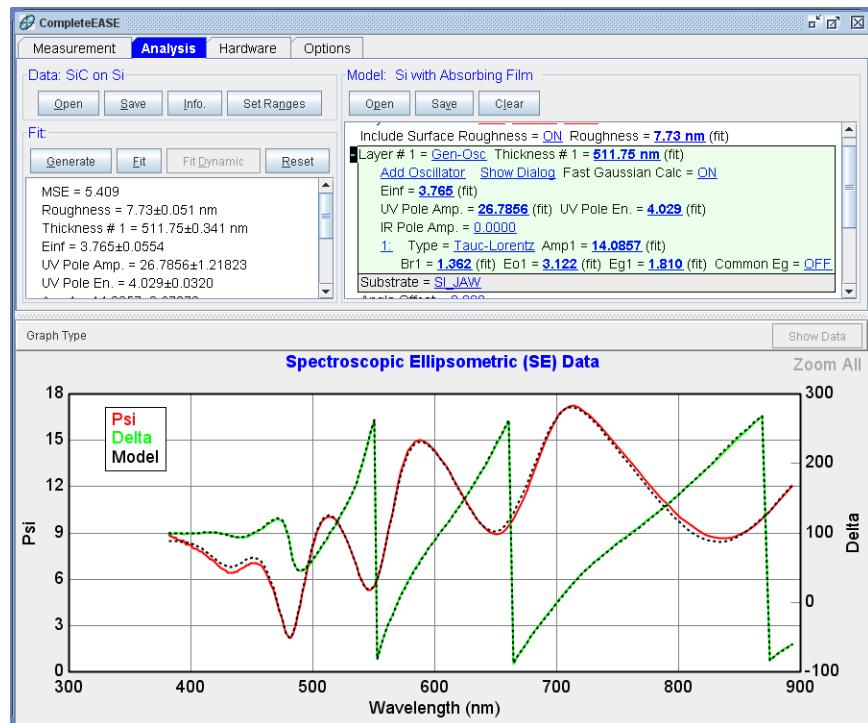


Figure 4-37. Gen-Osc has replaced B-Spline layer in the model.

## Glass with Absorbing Film

In this example, we will repeat the demonstrated procedures with an absorbing film deposited on glass substrate. In general, the data analysis is similar, with different substrate optical constants. Another consideration for transparent substrates is the possible presence of backside reflections. In this example, the backside of the glass substrate was mechanically roughened to avoid this extra complication. However, section 3.4 described methods to handle transparent substrates when backside reflections are present.

Open the “a-Si on Glass” data file and the “Glass with Absorbing Film” model, and click the ‘Fit’ button. The results should appear as shown in Figure 4-38. The “Absorbing Film on Glass” model uses the same procedures as previously described for the “Si with Absorbing Film” model. As before, the optical constants are described via a spline with equal spacing of 0.3 eV between nodes. This spacing can be changed for materials that exhibit stronger optical dispersion. The initial values are determined via a global fit of n and k with WVL-EXPAND fitting. To view the optical constants of the film, right-click the mouse on the “B-Spline” layer in the model and choose “Graph Layer Optical Constants”. The resulting “B-Spline” optical constants from the fit are shown in Figure 4-39.

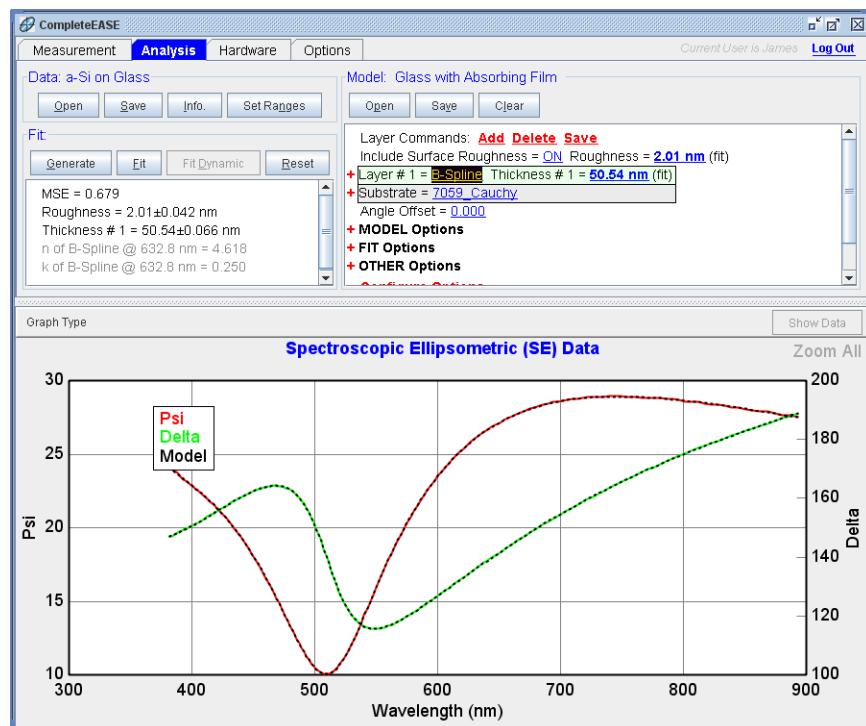


Figure 4-38. Results using “Glass with Absorbing Film” model to fit the “a-Si on Glass” data file.

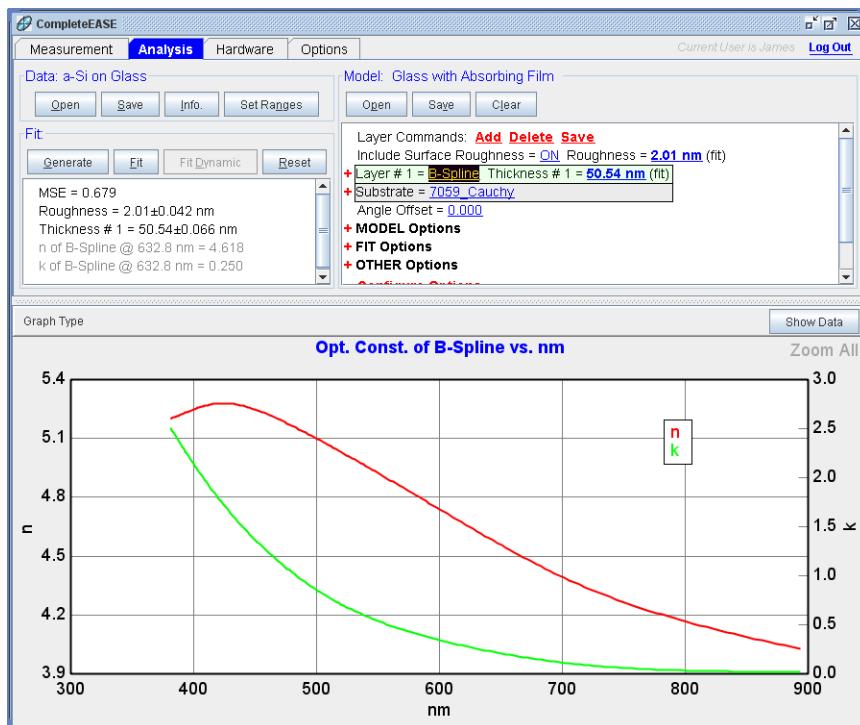


Figure 4-39. Resulting B-SPLINE optical constants for a-Si film.

## Starting Mat

The two models for absorbing films in this example are very flexible and can be used for many different materials. This is primarily due to the Global Fit of  $n,k$ . However, the data analysis takes longer than average, as the global fit attempts all possible combinations of  $n,k$  starting values. To minimize analysis time, the global fit range could be reduced. However, this would require knowledge of the appropriate range for the material. If the material is known, it is also possible to use a similar material file as the “Starting Mat” inside the B-SPLINE layer.

For best comparison of analysis time, re-analyze the “a-Si on Glass” data set using the “Glass with Absorbing Film” model. The analysis takes between 20 and 25 seconds on a Pentium D computer. Re-open the “Absorbing Film on Glass” model and make the following modifications:

- Expand the B-SPLINE layer and left-click “Starting Mat = none”. Open “a-si.mat” from the Semiconductor Folder.
- Turn OFF the global fit with **Model:>+FIT Options**.
- Press **Fit:>Fit**.

The data analysis should return the same result as before, but in less than one second. Thus, this new model would be an alternative for a-Si when the optical constants for the film are similar to the reference material file.

## Parameterizing Optical Constants with Cody-Lorentz

The a-Si optical constants can be parameterized, just as with the SiC values from the previous example. There are two common oscillators used for amorphous silicon: Tauc-Lorentz and Cody-Lorentz. To parameterize the B-Spline optical constants for the a-Si film in this example, right-click the B-spline layer and then choose “Parameterize Layer” from the drop-down menu.

The “Parameterize Layer” dialog box appears with the B-Spline layer optical constants plotted in the graph. The default for this layer is already set to a single “Cody-Lorentz” oscillator, so it is ready for this example.

As before, go through the three steps with the Gen-Osc parameterization, namely 1) match e2 using oscillator parameters, 2) match e1 with poles and Einf, and 3) match both and replace the layer. For step #1, there are two ways to manipulate the oscillator parameters by hand before “fitting”. As an exercise, vary the parameters manually.

1. Dial each oscillator parameter by holding the SHIFT key down while the mouse-wheel is rolled over top of the oscillator parameter. Holding CTRL-SHIFT will make reduce the step-size of each adjustment.
2. Left-Click ( $\text{Ctrl}+\text{L}$ ) on the number next to the Oscillator to highlight that oscillator. This shows “control” points on the graph that can be grabbed and adjusted with the mouse. Often, these control points are outside the measured spectral range, as in Figure 4-40. To view the control points of the oscillator, press the ‘Expand X-Axis’ button. This will widen the photon energy range to view the entire oscillator, as seen in Figure 4-41. Try adjusting the oscillator broadening, amplitude, and center energy by moving the gray control boxes on the graph. This will change the shape of the oscillator.

3.

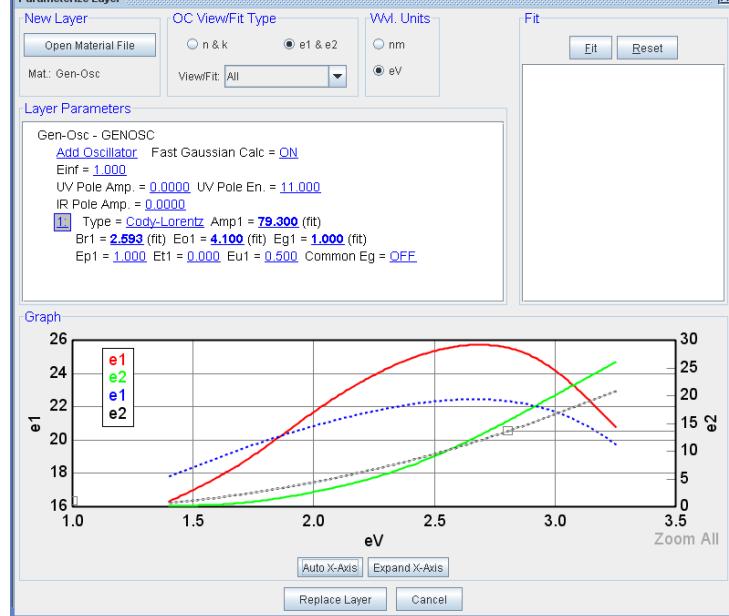


Figure 4-40. Click the number next to an oscillator to view the oscillator and its control points (in gray). As is often the case, the oscillator is outside the measured energy range, so it is difficult to locate.

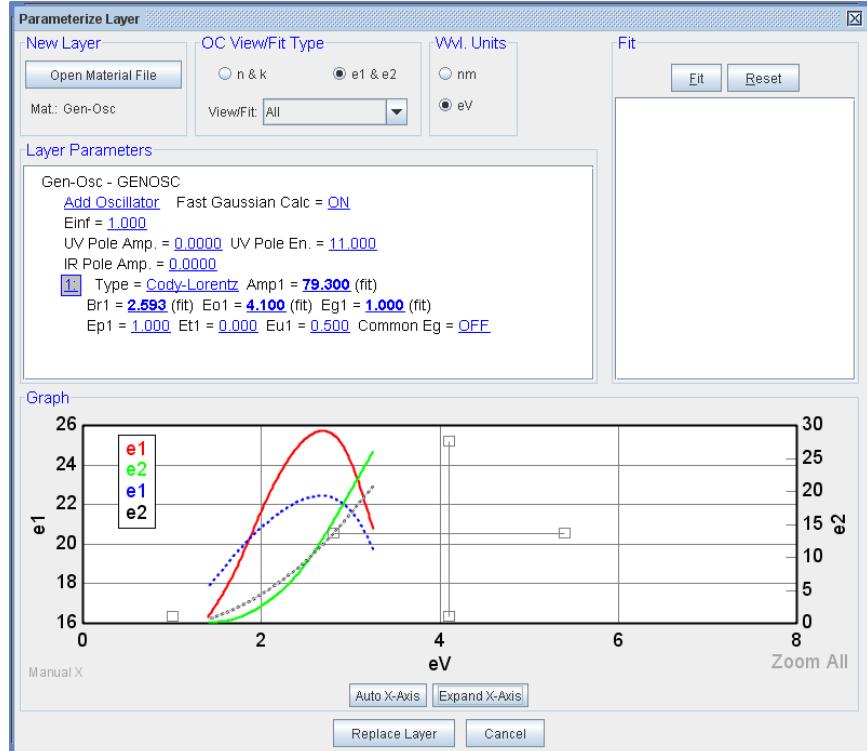
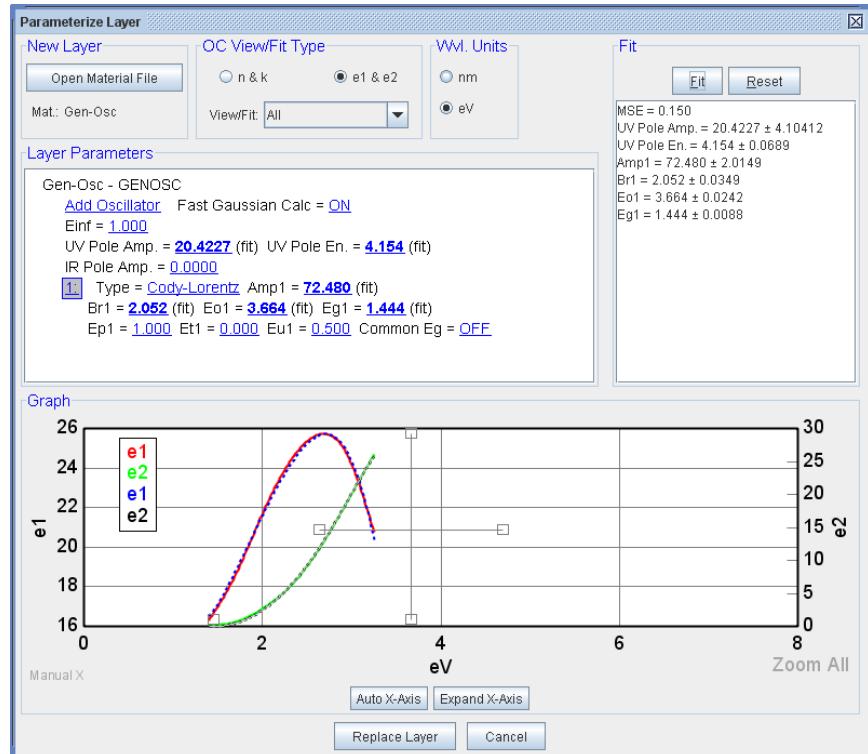


Figure 4-41. Press ‘Expand X-Axis’ to better view the oscillator and control points (in grey). The control points can be adjusted with your mouse to change the amplitude, center energy, broadening and bandgap for the selected oscillator.

Figure 4-42 displays the fit results; the black dashed curves in the graph are calculated using the specified oscillator. Go ahead and ‘Replace Layer’ to add this newly developed oscillator material file to the model. Fit the data and the result will have an MSE near 1.2.

Next, expand the oscillator layer in the model and add the following fit parameter to the fit: “Ep”. This allows added flexibility to the optical dispersion. The MSE should reduce to 0.8 as shown in Figure 4-43.

Add the additional fit parameters (Einf, Et, and Eu) to the model to check for further improvement. The question becomes whether slight MSE improvement warrants the increased number of “variables” in the modeling process. As a general “rule-of-thumb”, each additional fit parameter should decrease the MSE by 20% to make it a clear choice.



*Figure 4-42. Optical constants of a-Si from SPLINE fit are matched with a Cody-Lorentz oscillator.*

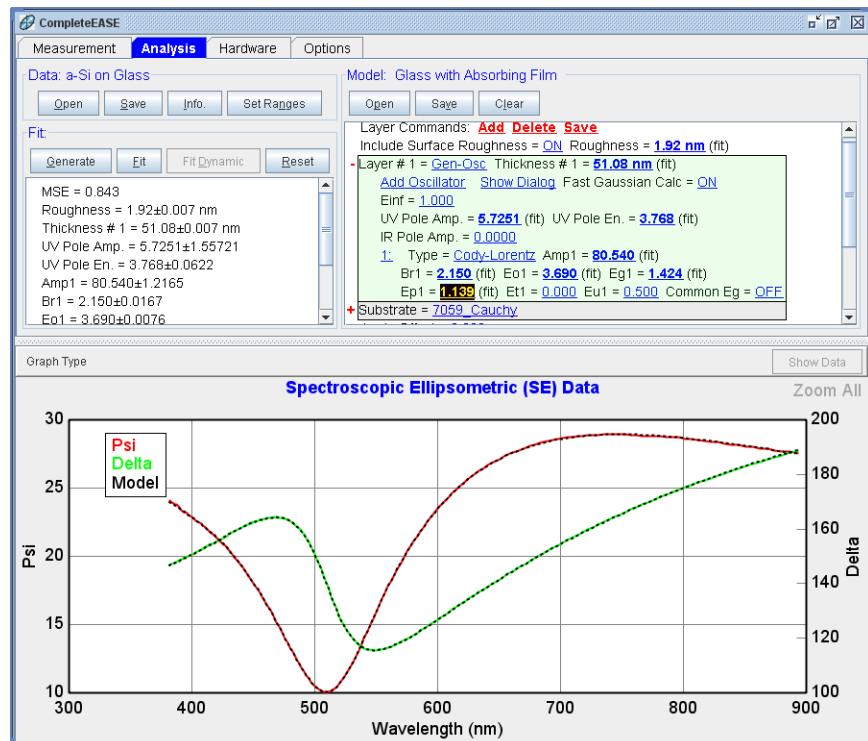


Figure 4-43. Final results using Cody-Lorentz oscillator to fit a-Si data set.

## Saving a Model

After the appropriate Cody-Lorentz fit parameters are determined for the a-Si film, the model can be saved for future use. This process is quite simple: press **Analysis>Model:>Save**. Choose the Folder where you would like to locate this model and give the model a name. The “Common” folder is a central location for easy access by all users. Figure 4-44 demonstrates this procedure.

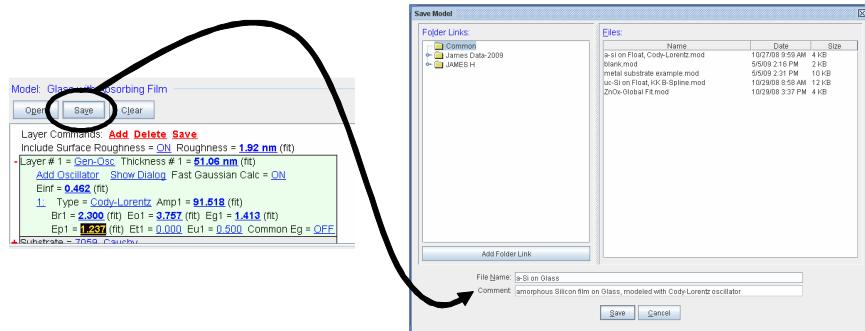


Figure 4-44. Press ‘Save’ from the **Model:** pane to bring up the “Save Model” dialog box.

## 4.5. Multiple Layer Film Stacks

### NEW FEATURES IN THIS EXAMPLE

- Modifying a Model
- Global Fit/Pre-Fit with multiple layers

Open the data file “a-Si Multilayer”. This sample is similar to those discussed in Section 4.4. The substrate is silicon with a SiO<sub>2</sub> film underneath the a-Si. No model exists for this type of sample, so it will need to be constructed. It is preferred to start by modifying a similar model. Let’s start with the model saved in Section 4.4 for a-Si on glass using a Cody-Lorentz oscillator. Open this model from the “Common” location. If you did not save the model, then repeat Section 4.4 before proceeding and make sure to save the final model as suggested.

NOTE: Make sure to replace the substrate with silicon.

Left-click on the “7059\_Cauchy” layer and open “Si\_Jaw” from the Semiconductor location of the Open Material dialog box.

Select the **Add** command from the top of Model pane. This will bring up the dialog box shown in Figure 4-45. Move the mouse to locate the Blue bar between the two current layers (as shown). This will be the location of the newly added layer. Choose “SiO<sub>2</sub>\_Jaw” from the Semiconductor location of the Open Material dialog box.

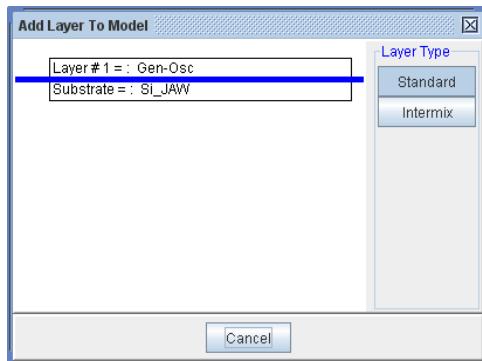


Figure 4-45. The **Add** command opens the dialog box shown. The blue bar can be moved up or down to designate the location of the added layer.

Left-click the “Thickness #1= 0.00nm” designation for the SiO<sub>2</sub> layer to change its thickness to a nominal value of 100nm. Also select this thickness as a fit parameter. Generate data and the graph should appear as shown in Figure 4-46. The generated data does not match the experimental data. If a fit is attempted from this point, it will not be successful. Press Fit.

Press CTRL-R to **reset** the model to the previous values after verifying the poor fit quality.

The poor fit is due to the unknown thickness values. There are a couple approaches to determine better starting thickness values for each layer. Both approaches work better if the Cody-Lorentz oscillator parameters are turned OFF before proceeding:

- Expand General Osc layer and right-click on each of the fit parameters that was previously turned on, toggling them off.

Three layer thicknesses remain as fit parameters (SiO<sub>2</sub>, a-Si, roughness).

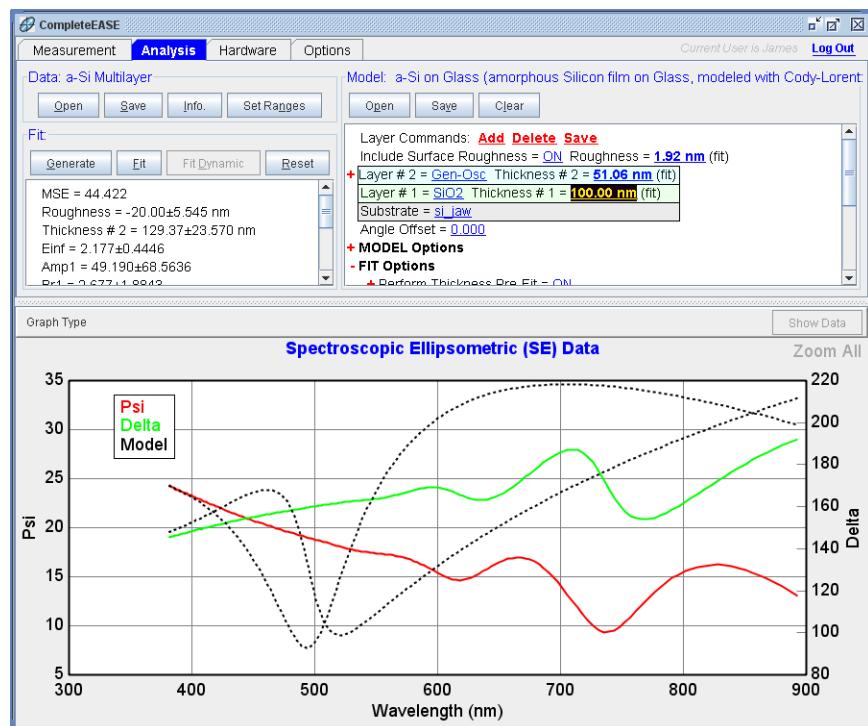


Figure 4-46. Generate data with a nominal thickness of 100nm for SiO<sub>2</sub> layer.

**Approach #1:** Use a Global fit for both Thickness #1 and Thickness #2. Make sure to turn off the Thickness Pre-fit. This method can take a very long time if the search includes a wide range of possible thicknesses.

**Approach #2:** Use the Global fit for the SiO<sub>2</sub> layer thickness with the Thickness Pre-fit turned on. This reduces the global fit dimension and works much more quickly.

NOTE: Approach #2 will not work if the a-Si layer (Thickness #2) is used within the Global Fit rather than the SiO<sub>2</sub> layer (Thickness #1). The Thickness Prefit always operates on the thickest layer in the model.

Figure 4-47 shows the successful fit of the sample. The current model does not include the oscillator parameters, so the a-Si film must have similar optical constants to the previous sample.

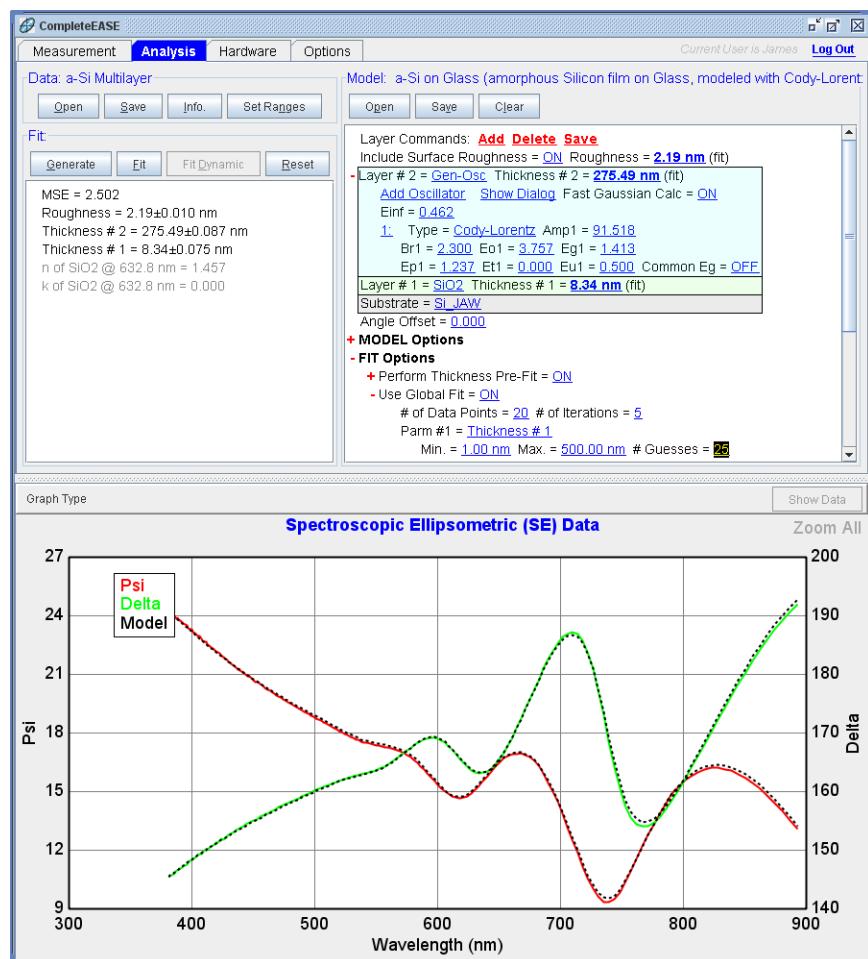


Figure 4-47. Fit result for Layer Thicknesses only.

- Include Derived Parameters = ON
- [Add Derived Parameter](#)
- 1. Type = n Layer # = 2 Wavelength = 632.8 nm Name = n of Gen-Osc @ 632.8 nm  
Low Spec. = 0.000 High Spec. = 0.000
- 2. Type = k Layer # = 2 Wavelength = 632.8 nm Name = k of Gen-Osc @ 632.8 nm  
Low Spec. = 0.000 High Spec. = 0.000

Figure 4-48. The Fit Options section of Model pane allow Derived Parameters to report the optical constants from any layer in the model. With multilayer films, the correct layer # must be entered.

The Cody-Lorentz parameters can now be turned on to improve the fit quality by allowing the a-Si optical constants to vary. Figure 4-47 also points out that the Derived Parameters are pointing to the wrong layer number. Within the Fit Options section of the Model pane, change the Layer number from #1 to #2 for both the Derived *n* and Derived *k* as shown in Figure 4-48.

Add the Cody-Lorentz parameters back as fit parameters (right-click on their values). Turn off the Global Fit and Thickness Prefit (as the thicknesses are already well known) and press the ‘Fit’ button. The results should appear as shown in Figure 4-49. Save the new model for future use on similar samples.

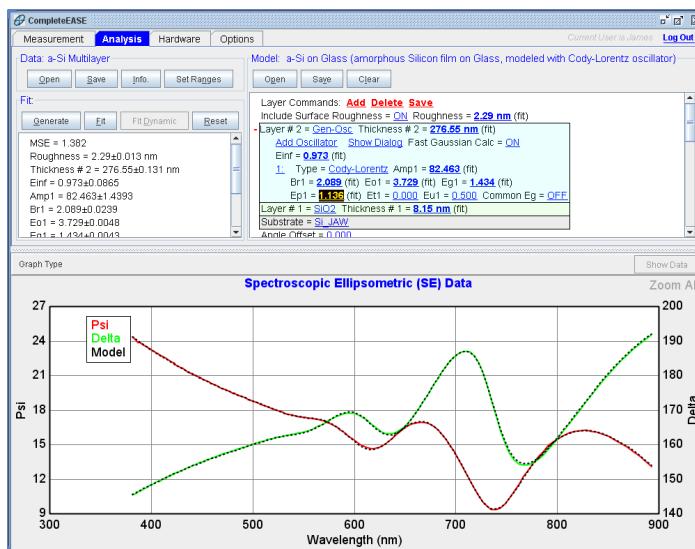


Figure 4-49. Final fit results for a-Si multilayer.

## Oxide or Roughness?

There is often a question whether the surface is oxidized or rough. In the model above, surface roughness was implemented with a final value of 2.29 nm. Turn the roughness off and AddLayer of “SiO<sub>2</sub>\_Jaw” on top of Layer #2. Fit the data. The final result should have SiO<sub>2</sub> surface layer of 2.70nm with an MSE of 1.25. Thus, there is very little difference between roughness and oxide for this sample. This is true in general when the film thickness is below about 10nm. In the case of Silicon, it is more likely the surface is oxidized than rough, but both models work.

## 4.6. Multiple Data Types (SE + T)

| NEW FEATURES IN THIS EXAMPLE  |   |
|-------------------------------|---|
| • Appending Data              | • Fitting SE and Transmission data simultaneously |
| • <b>Parameter Uniqueness</b> | • Graph ScratchPad                                |

A common approach to increase the information content when measuring absorbing thin films on transparent substrates is to supplement the SE data with Intensity Transmission data. This extra information can help insure a unique result for thickness and optical constants of the thin absorbing layer.

As a demonstration, open the “Cr on glass\_SE” data file from the EXAMPLES folder. This data was collected from a thin Cr film on glass, with the backside taped to suppress backside reflections. Therefore, we can open the “Glass with Absorbing Film” model. This model was described in an earlier example and is designed for films that may be nearly transparent at longer wavelengths, but exhibit UV absorption. While this model will likely work without modification for the metal on glass, there is a better approach to start. Perform the following before pressing fit:

- Turn off the Surface Roughness.
- Turn off the Global Fit under the **+Fit Options**
- Choose the Cr.mat file from the metals directory as the “starting mat=” inside the B-Spline layer.

### **Parameter Uniqueness**

Now, you are ready to press ‘Fit’. Your initial result should look similar to that shown in Figure 4-50. Because there is large correlation, pressing fit again-and-again will result in different results with nearly the same low MSE. To visualize the MSE profile, use the **Parameter Uniqueness** option under the **+OTHER Options** section of the model. Figure 4-51 shows the results for a Parameter Uniqueness test of the thickness from 10nm to 50nm. Before proceeding, copy this curve to the Graph ScratchPad for later comparison. Although there is a minimum value for the MSE around 45nm, the MSE value is below 0.4 for most of the thickness range.

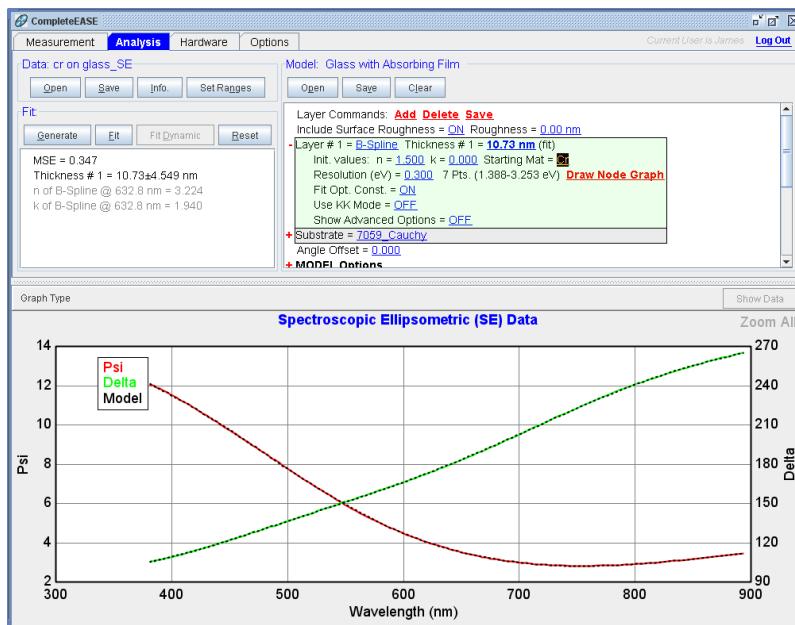


Figure 4-50. Starting fit to only the SE data using a B-Spline layer.

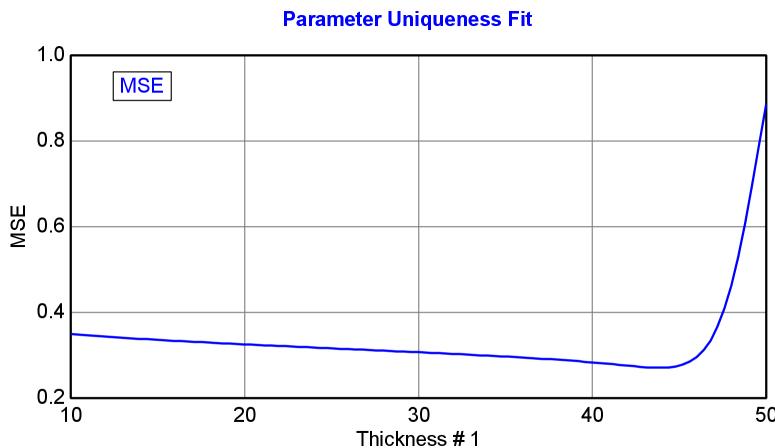


Figure 4-51. MSE profile from the Parameter Uniqueness test of thickness when only fitting the SE data for a Cr film on glass.

## Append Data

To help break this correlation apparent when only fitting the SE data, let's add the Intensity Transmission to the fit to provide additional information. We want both the SE data and the Transmission Intensity data present in the fit. To this end, you need to right-click (**Ctrl**) on the 'Open' data command and select "Append Data" as in Figure 4-52. Choose to append the "Cr on glass\_T" data file from the EXAMPLES directory. This data was collected from the same sample. With both data files present, you can switch between graphs of SE and T data by choosing the data set right above the graph, as shown in Figure 4-53.

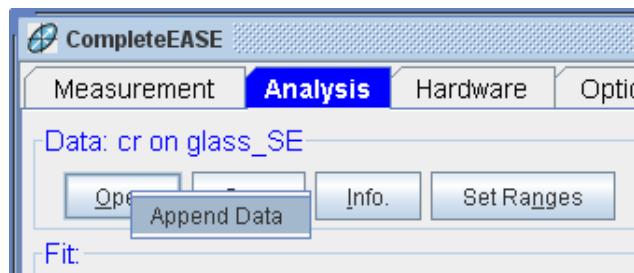


Figure 4-52. Right-click on the ‘Open’ command to choose “Append Data” when adding Transmission data to the already opened SE data.

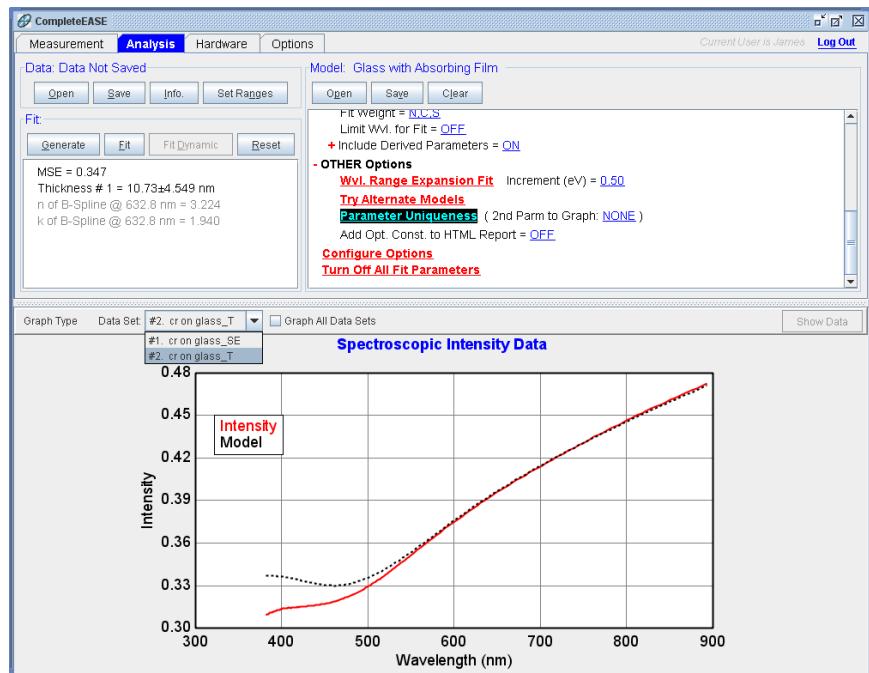


Figure 4-53. Choose the data set to graph by selecting entry just above the graph. Here, you can see that both SE and T data for the Cr on Glass sample are open simultaneously. Thus, they will both be included in the fit.

## Transmission Data % Weight

Anytime Transmission Intensity data is fit, you should check the “Transmission Data % Weight”. This is the value that tells CompleteEASE how to weight the Transmission compared to Spectroscopic Ellipsometry data. Most models will have this value set to 100%, so the Transmission Intensity has equal weighting to the Spectroscopic Ellipsometry data. However, certain models can be saved with values other than 100%. To view the “Transmission Data % Weight”, you will need to press the **Configure Options** button at the bottom of the Model. In the Fit Options section, check the “Transmission Data Weighting” option, as shown in Figure 4-54.

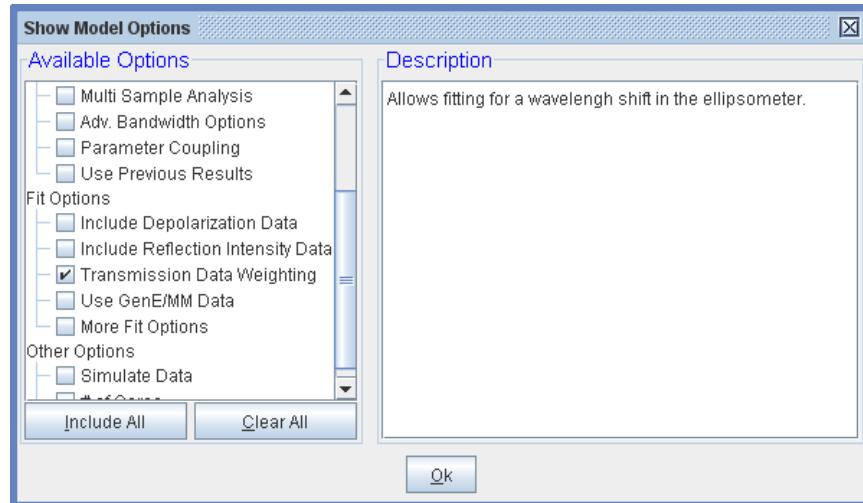


Figure 4-54. Adding the “Transmission Data Weighting” option from the [Configure Options](#) section of the Model.

After turning on the Transmission Data Weighting, you will need to set this value to 100% in the Fit Options section of the Model, as shown in Figure 4-55.

#### + MODEL Options

##### - FIT Options

- + Perform Thickness Pre-Fit = [ON](#)
- Use Global Fit = [OFF](#)
- Fit Weight = [N.C.S](#)
- Transmission Data % Weight = [100.00](#)
- Limit Wvl. for Fit = [OFF](#)
- + Include Derived Parameters = [ON](#)

Figure 4-55. Change the “Transmission Data % Weight” to 100% in the +Fit Options section of the Model.

Go ahead and press ‘Fit’ again. If the model thickness starts close to the correct answer, the fit should find a thickness near 14nm. This is the final result. However, if the Cr thickness is started too far away from 14nm, the fit can get stuck in a “local” MSE minimum. Repeat the Parameter Uniqueness test to check the MSE profile, which should produce a curve as shown in Figure 4-56. It is obvious that there is only a single thickness that will provide the best MSE, although we can also easily see how it is possible to get stuck in the “local” minimum near 45nm.

Again, copy this curve to the Graph ScratchPad. Now, we can compare the MSE profiles from the previous two Parameter Uniqueness tests by viewing the Graph ScratchPad, as shown in Figure 4-57.

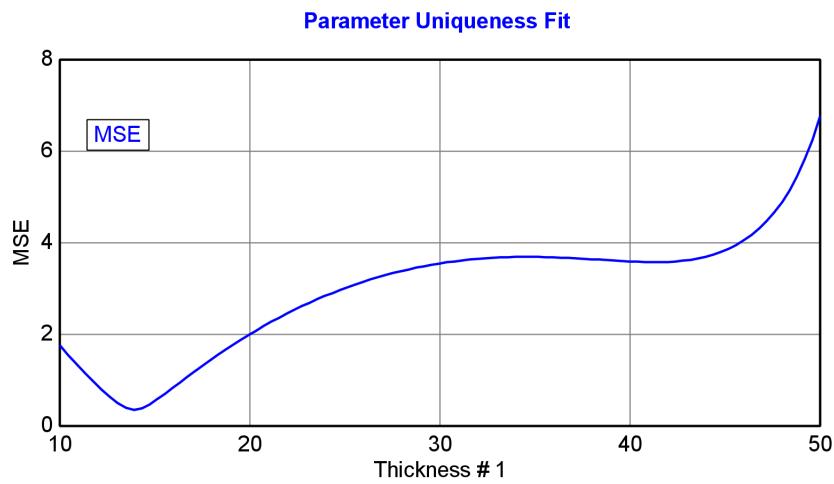


Figure 4-56. MSE profile when fitting both SE and T data simultaneously for a thin Cr layer on Glass.

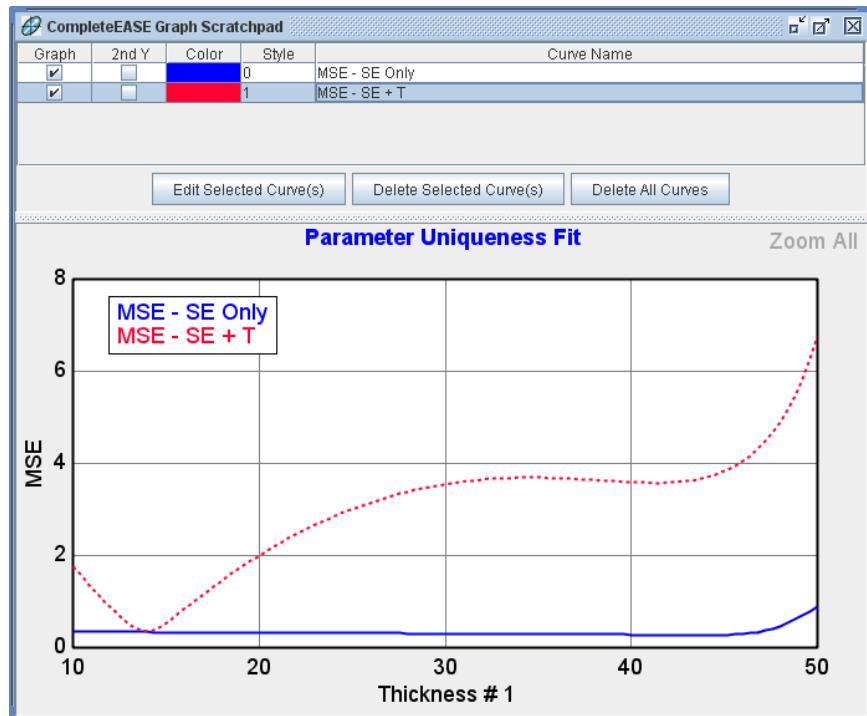


Figure 4-57. Graph ScratchPad comparing the MSE profile when fitting both SE and T data or only the SE data from a thin Cr layer on glass.

# 5. Data Analysis 3 – Advanced

This chapter includes further examples to demonstrate both advanced and specialized topics. Advanced topics include multi-sample analysis, creation of composition and temperature dependent material files and working with anisotropic or non-ideal models. A few of the examples use data from mapped samples, which help demonstrate how to work with data collected at multiple points from a sample. However, not all ellipsometers have this capability, so modeling of mapping data is only necessary for specific systems.

The section examples from this chapter are listed below, along with the primary CompleteEASE features that are discussed.

## Section 5.1 Map Data and Model Non-Idealities

| FEATURES IN THIS EXAMPLE   |   |
|--|---|
| <ul style="list-style-type: none"><li>• Show Map Data</li><li>• Selecting single-points from Map</li><li>• Sellmeier Layer</li><li>• Thickness Non-Uniformity</li><li>• Set Ranges</li></ul> | <ul style="list-style-type: none"><li>• Fit Scan Data</li><li>• Viewing Map Results</li><li>• Model Calculation (Non-idealities)</li><li>• Bandwidth (nm)</li></ul> |

## Section 5.2 Multi-Sample Analysis

| FEATURES IN THIS EXAMPLE   |  |
|--|--|
| <ul style="list-style-type: none"><li>• Selecting Multiple Points from Map</li><li>• CTRL-SPACE BAR to switch views.</li><li>• Set Symbol Size</li><li>• Graph All Data Sets</li><li>• Multi-sample Analysis</li></ul> | <ul style="list-style-type: none"><li>• Model: Multi-layer (empty)</li><li>• Select/Un-Select Data Set</li><li>• Zoom on “Map”</li><li>• Clear Multi-Data Set Mode</li><li>• Add Fit Parameter</li></ul> |

### Section 5.3 In Situ Data Analysis

#### FEATURES IN THIS EXAMPLE

- |  |                                |
|--|--------------------------------|
| • Viewing individual time-slices                   | • ‘Dynamic Fit’                |
| • Selecting multiple-time slices from dynamic scan | • Multiple-Time Slice Analysis |

### Section 5.4 Creating OC Library for Composition or Temperature-dependent materials

#### FEATURES IN THIS EXAMPLE

- |  |  |
|--|--|
| • Creating composition or temperature dependent material files | • OC Library Mode                      |
| • Opt. Const. Compare Model<br>(OC Compare)                    | • <a href="#"><u>Build Library</u></a> |
| • <a href="#"><u>Draw Graph</u></a>                            |  |

### Section 5.5 Anisotropic Films

#### FEATURES IN THIS EXAMPLE

- |                          |                   |
|--------------------------|-------------------|
| • Convert to Anisotropic | • Difference Mode |
| • Biaxial Layer          |                   |

## 5.1. Map Data and Model Non-Idealities

| FEATURES IN THIS EXAMPLE           |                                      |
|------------------------------------|--------------------------------------|
| • Show Map Data                    | • Fit Scan Data                      |
| • Selecting single-points from Map | • Viewing Map Results                |
| • Sellmeier Layer                  | • Model Calculation (Non-idealities) |
| • Thickness Non-Uniformity         | • Bandwidth (nm)                     |
| • Set Ranges                       |                                      |

For this example, we will open a data file that contains multiple points scanned across a silicon wafer with thick SiO<sub>2</sub> coating. Our goal is to effectively determine the SiO<sub>2</sub> thickness and refractive index, along with the uniformity of the thin film properties across the wafer.

### Show Map Data

Open the data file “SiO<sub>2</sub>\_Map” from the EXAMPLES folder. You should see a color image of the Psi data across the center of a circular sample. To better understand what is shown, right-click on the graph panel and check “Show Symbols”. This will mark the individual measurement locations, as in Figure 5-1. This uniformity map was created from a Radial scan of the wafer. We can visualize the uniformity of the ellipsometry parameters, but need to first analyze the data before we can visualize the thin film properties of interest.

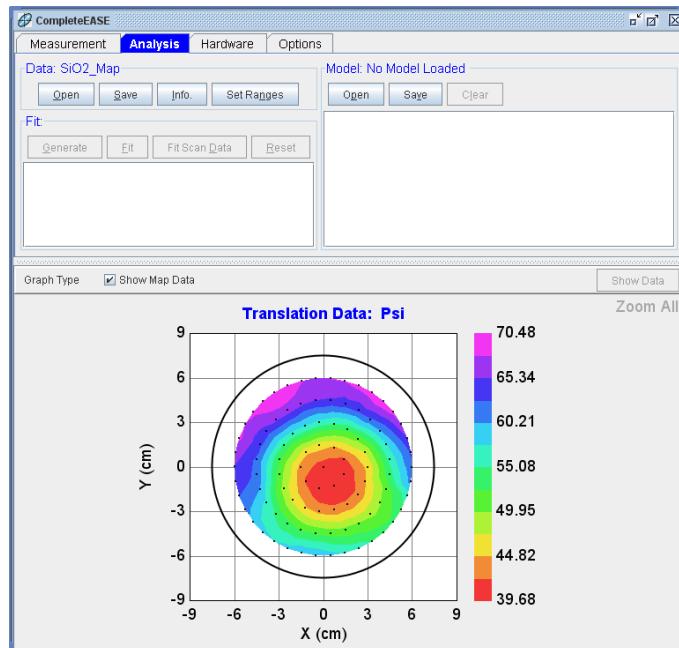


Figure 5-1. Map Data for “SiO<sub>2</sub>\_Map” data file. With symbols shown, we can visualize each point on the wafer that was measured.

## Selecting a Point from the Map

If you press your left mouse button on any of the points of the map, it will load the spectroscopic ellipsometry data from that single location into the graph. This is a convenient way to choose a point to help construct a model to analyze the map. Go ahead and select a point with your mouse. The graph will change to Psi/Delta, as in Figure 5-2. Notice that an additional option is available at the top of the Graph Pane: “Show Map Data”. This allows you to go back to the colorful map of Psi and Delta.

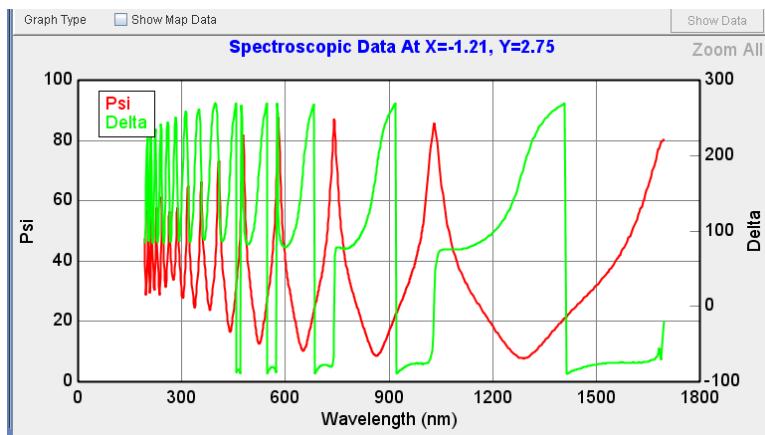


Figure 5-2. Spectroscopic Data from a single-point of the map. This view was gained by left-clicking the mouse on a map point.

## Silicon with Transparent Film

While this film is  $\text{SiO}_2$ , it is not necessarily a thermal oxide. Therefore, choose the “Silicon with Transparent Film” model that was first described in Section 3.3 for an unknown transparent layer. Go ahead and open this model and press ‘Fit’ which runs the model to fit the SINGLE point that is selected.

Before fitting all points on the map, we need to turn off the “Global Fit”, or the fit will take a very long time. The fit result should appear similar to Figure 5-3. The MSE is rather large which suggests there is a problem with this model. Thick films have a large number of interference oscillations, especially at short wavelengths. On this scale, it is difficult to see whether our model is adequate over the full spectrum.

## Wavelength Units – eV

To better view short wavelengths, go ahead and convert the graph “Wavelength Units” to photon energy (eV) instead of nm. This will expand the UV region to give near-equal spacing between the interference oscillations. Wavelength and photon energy are inversely related. Thus, large photon energies are actually the shortest wavelengths. To convert to photon energy, either use the short-cut CTRL-ALT-W or go to the **Options** tab and change the Wavelength Units to eV within the **Display Units** pane. Figure 5-4 shows the data and model versus photon energy. For simplicity, I have turned off the Double-Y axis for the graph. It is now very clear that the short wavelengths (high eV) are not matched by the model. This is a problem with the final Cauchy parameters that were found.

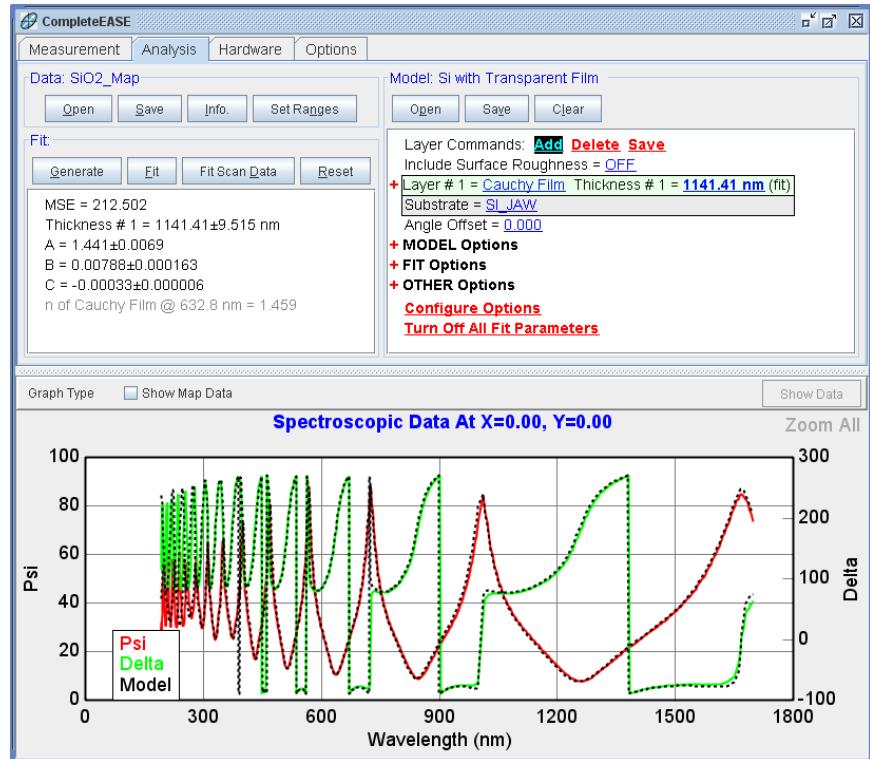


Figure 5-3. Fit results for a single-point of the SiO<sub>2</sub> map using the “Silicon with Transparent Film” model.

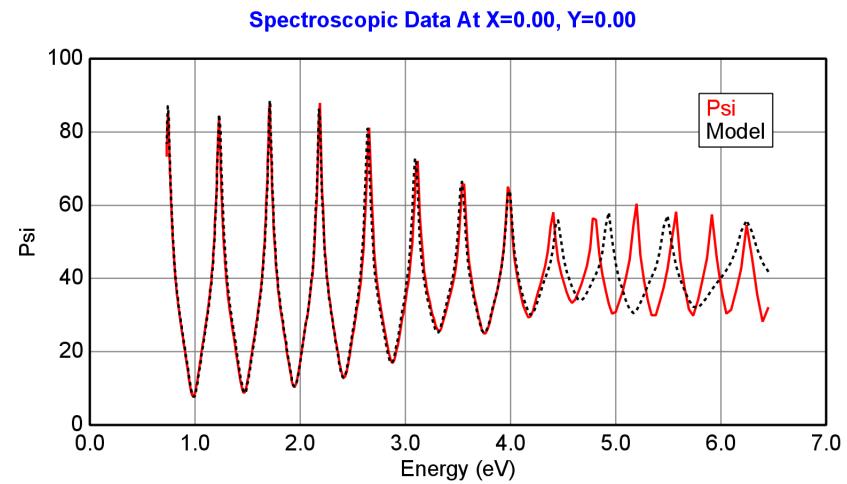


Figure 5-4. Data fit for Psi shown versus photon energy (in eV) to better visualize the discrepancies at short wavelengths (large eV).

## Fixing Cauchy Dispersion

The Cauchy parameters work well to describe the index of refraction in the transparent region, but the Cauchy does have some limitations. It was not intended to cover very wide spectral ranges and it does not necessarily maintain a “physical” shape. The Cauchy parameters appear to fit the data well until about 4.5 eV. Above this range, there is not enough dispersion to match the correct interference oscillations. To fix this problem, we can either redo the fit with the B and C terms of the Cauchy included in the Global Fit (which will take a very long time) or range-select the region that is fit and slowly add more wavelength range. The second approach is demonstrated. First, range-select the data up to about 4.5 eV. Turn off the Global Fit and Thickness Pre-fit. They are no longer needed, as we are close to the final model. Press ‘Fit’. The Cauchy parameters will adjust to better match this range. Your result should look similar to those shown in Figure 5-5.

For this example, do not worry about matching the manual results exactly, as you may have selected a different point from the uniformity map.

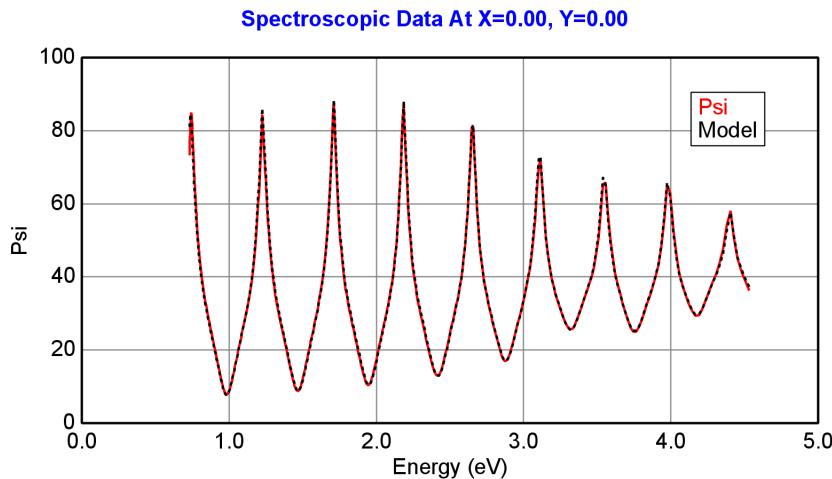


Figure 5-5. Cauchy fit to 4.5eV.

## ‘Set Ranges’

Next, extend the data range to 5.0eV. To add this extra range, let’s try using the **Data: > ‘Set Ranges’** command. This will allow you to type in the new MAX photon energy. The ‘Set Ranges’ dialog box is shown in Figure 5-6. After selecting up to 5eV, press ‘Fit’. Keep adding extra photon energy in 0.5eV increments and fitting the data until you have all data graphed. The final fit should appear as in Figure 5-7. The MSE is significantly improved – near 40 – compared to the previous MSE of over 200.

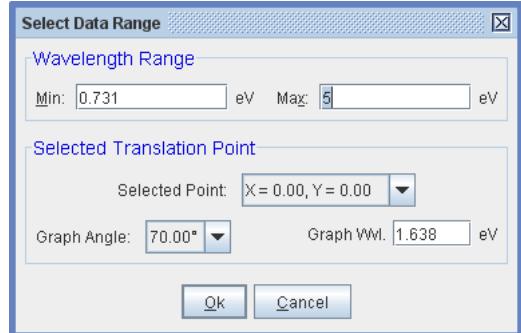


Figure 5-6. ‘Set Ranges’ command allows you to set the wavelength range and choose which data point you have selected.

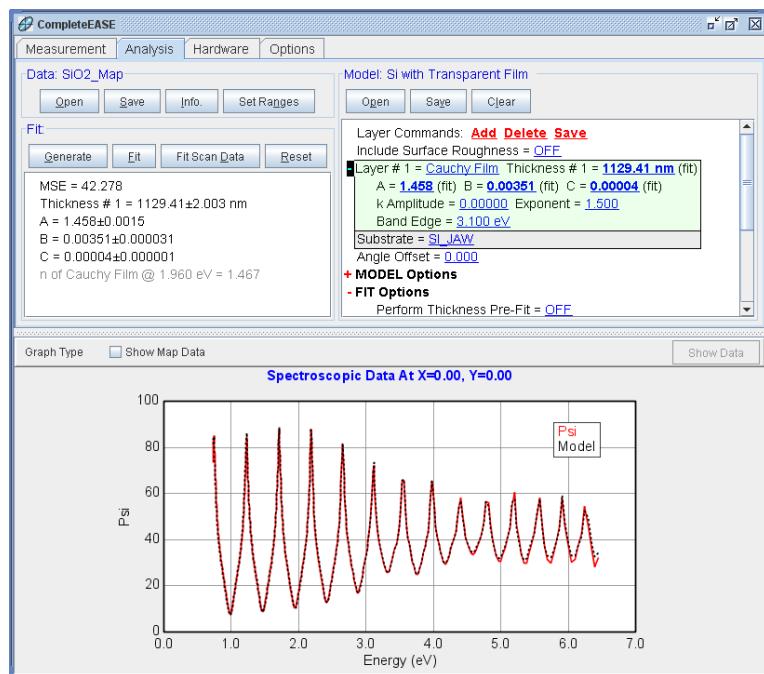


Figure 5-7. Final fit to all wavelengths using Cauchy dispersion.

## Sellmeier

Although we are able to get the Cauchy to better match the data with a little work, it is not designed to handle such a wide spectral range. A better model for transparent films that cover a wide spectral range is the Sellmeier relationship. It has the added benefit of remaining Kramers-Kronig consistent – thus ensuring “physical” shape for the resulting index of refraction.

Replace the Cauchy layer in your model by pressing the Cauchy name with left-mouse click and go to the Dielectrics directory. Choose “SiO2 (Sellmeier)” material file in place of the Cauchy. Press ‘Generate’ and the starting point should be close to the experimental data, as in Figure 5-8. Go ahead and fit the SiO2 thickness and all four Sellmeier parameters. Your MSE should be near 30 (as compared to values as high as 200 and as low as 40 with the Cauchy). Thus, this model better matches the true shape of SiO2 index dispersion over a wide spectral range.

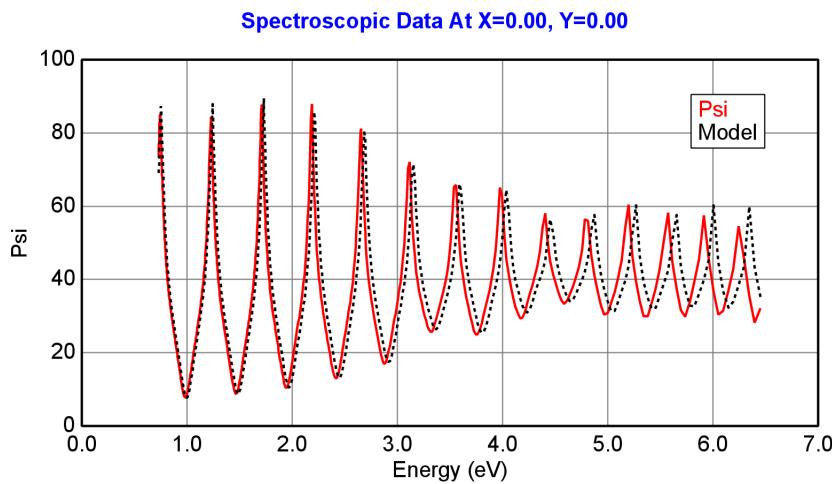


Figure 5-8. Generated data with the Sellmeier model for SiO<sub>2</sub> (before fitting).

## Fit Scan Data

Now that we have “tuned” the model for a single point from the map, we are ready to fit data over all points. Make sure to simplify the model by turning OFF:

- the Thickness Pre-Fit and
- the Global Fit

Both options are found in the **+FIT Options** section of the Model. After both are turned off, press the “Fit Scan Data” from the **Fit:** panel.

If you leave the thickness prefit and global fit ON during analysis of a full scan, it will take excessively long. However, if there are large variations across the sample, these may need to be turned back on – using caution and narrowing the search range of a Global fit.

After the data from all points are analyzed, their results will be shown in the **Fit:** panel, as in Figure 5-9. Now, if you press your left-mouse button on any of the “blue” parameters, the graph will update with uniformity map of that parameter. As an example, the Thickness #1 parameter is graphed, as shown in Figure 5-10.



Figure 5-9. Scan Data results are shown in the Fit: panel. Press any of the “blue” parameters in this list to view the map of that parameter.

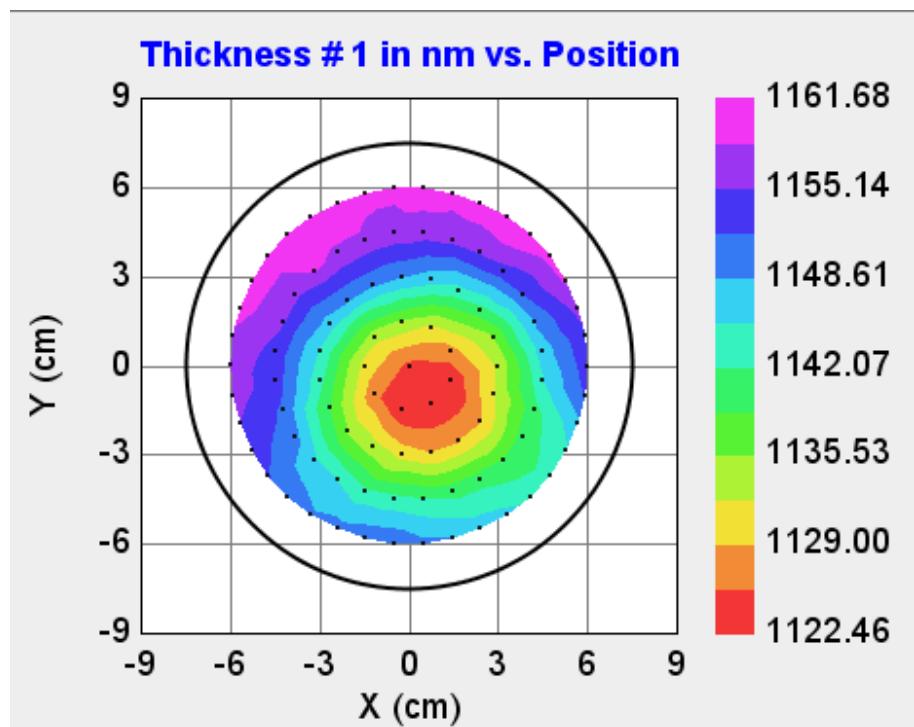


Figure 5-10.  $\text{SiO}_2$  thickness uniformity map.

## Model Calculation

Now, let's return our attention to the fit at a single-point. Try pressing a point on the Thickness map and you will find that the "results" maps do not allow you to jump directly to the data. Therefore, we first need to switch the graph back to Psi or Delta. To do this, simply check the "Show Map Data" box at the top of the Graph panel. After the graph is switched, go ahead and left-click your mouse on a point toward the center of the graph. Again, the spectroscopic data from that point is graphed and automatically fit with our model.

Psi and Delta are matched reasonably well. However, there may be more information about this sample to consider. Take a look at the depolarization curve, which was NOT currently included in the MSE calculation. Press CTRL-Z to see a depolarization graph as shown in Figure 5-11. The increasing depolarization toward short wavelengths (large eV) is very common for thick layers. The cause of this depolarization is due to a non-ideal consideration. The most common non-idealities for thick layers are thickness non-uniformity or instrument bandwidth. Both can be included in our model.

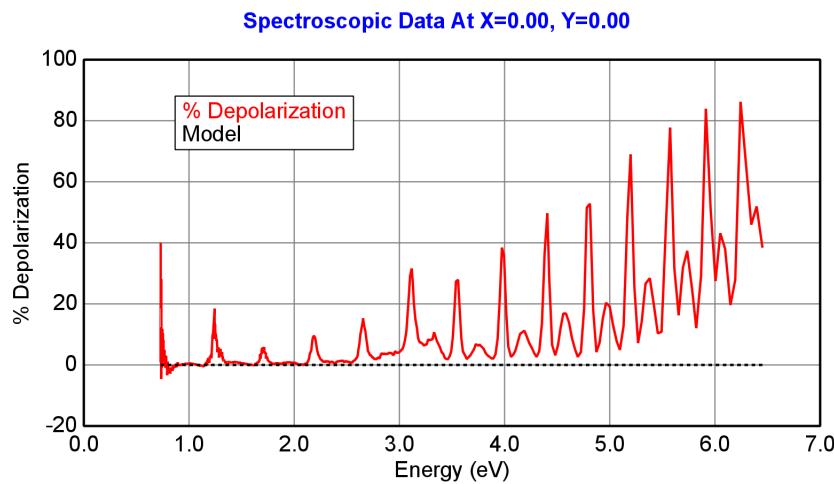


Figure 5-11. Depolarization curve for the thick SiO<sub>2</sub> film.

## Model Calculation – Thickness Non-Uniformity

Go to the **+MODEL Options** section of the Model and change the “Model Calculation” from “Ideal” to “Include Thickness Non-uniformity”, as shown in Figure 5-12. This will calculate the effect on the data points if there was a thickness variation within the measurement spot. Unless the system used a focused beam, this is a valid possibility. Hold the SHIFT key down and roll your mouse button up/down over the Thickness Non-Uniformity value. When you get to 2.4%, the model curve will better match the experimental depolarization, as shown in Figure 5-13. This value can be fit – right click on the thickness non-uniformity and fit the data. The MSE should reduce down below 20 (as compared to near 30 without thickness non-uniformity). This is due to improvement in the Psi/Delta fits, as we are not including the Depolarization data as part of the MSE calculation yet.

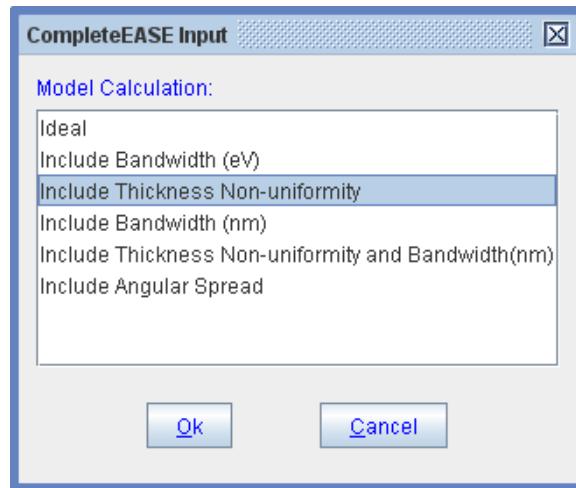
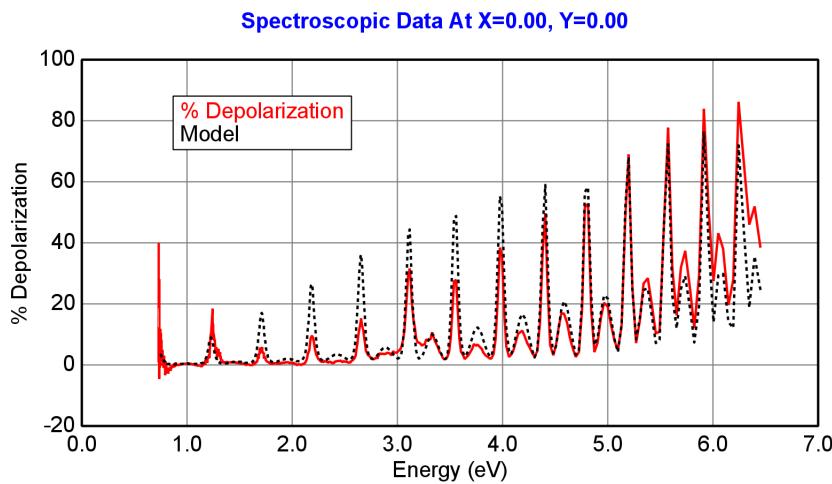


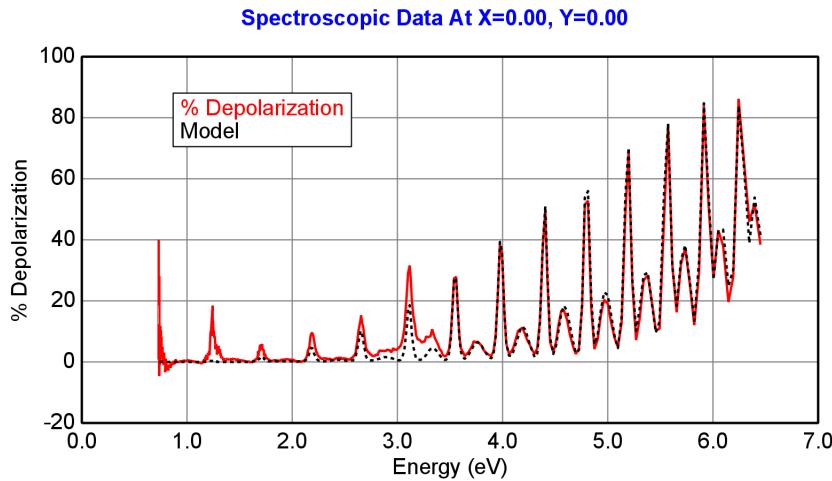
Figure 5-12. Model Calculation choices.



*Figure 5-13. Depolarization data with 2.4% Thickness Non-uniformity in model calculation.*

## Model Calculation – Bandwidth (nm)

Next, try changing the “Model Calculation” to “Include Bandwidth (nm)”. SHIFT-ROLL your mouse until the starting value matches the depolarization data. Then, fit for the Bandwidth. The result should have an even better MSE than with Thickness Non-Uniformity. The depolarization data are matched even better, as shown in Figure 5-14. This is due to the spectral differences between bandwidth and thickness non-uniformity. Thus, this model calculation appears to be the best. This is further verified by the final result that shows Bandwidth near 4nm, which is physically true for the M-2000 used for these measurements.



*Figure 5-14. Depolarization data fit with Bandwidth calculated in model.*

## Include Depolarization Data

Thus far, we included Model Non-idealities to better match the depolarization data, but the depolarization data were not included in the MSE calculation. Thus, we have shown that the non-idealities will also better match the shapes of Psi and Delta (as the MSE was reduced). Now, we include the depolarization data in the MSE calculation. To do this, press the **Configure Options** menu at the bottom of the Model. This feature is hidden. Under Fit Options section, check the “Include Depolarization Data” choice, as shown in Figure 5-15. Press ‘Ok’. Now, we must turn this feature on in the +FIT Options section. After turning on the “Include Depolarization Data”, press ‘Fit’ again. The MSE should be further reduced, while the bandwidth stays close to where it was without including the depolarization data. As a final step, re-fit all points of the map. Press ‘Fit Scan Data’ and you should get resulting maps similar to those in Figure 5-16, Figure 5-17, and Figure 5-18.

Analysis time is much longer when Model Non-Idealities are included. You will notice the analysis of all mapped points takes considerable time now that we include the Bandwidth.

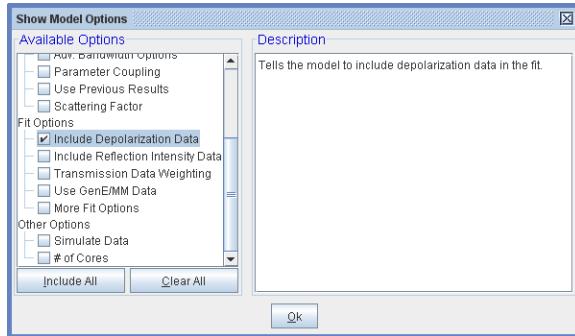


Figure 5-15. Press **Configure Options** to select hidden menu “Include Depolarization Data”.

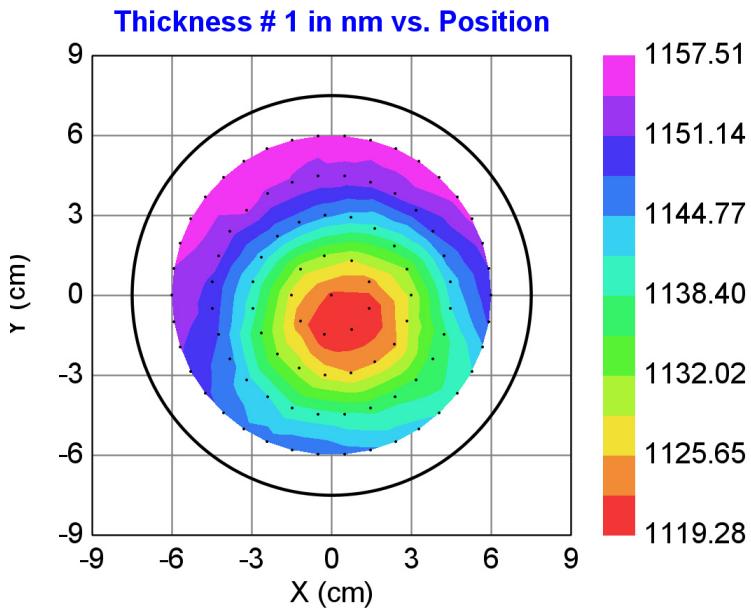


Figure 5-16. Final Thickness Map using Sellmeier model and including the Bandwidth.

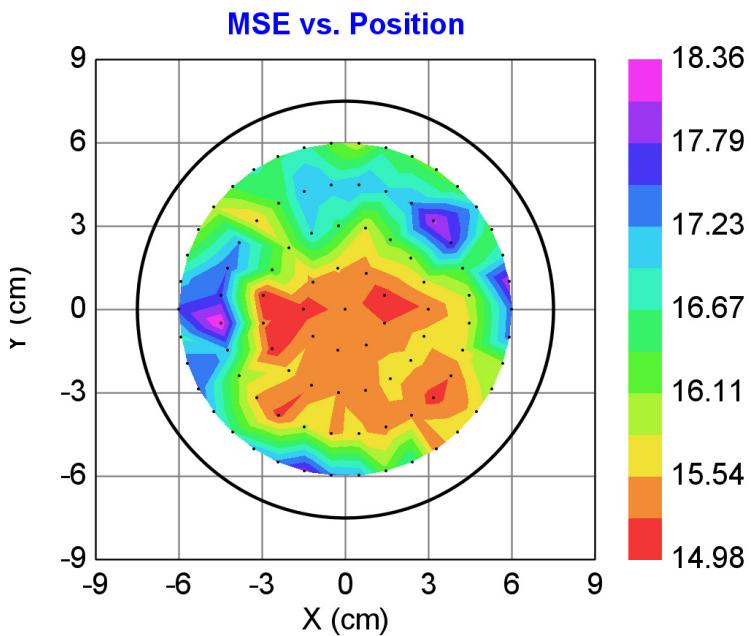


Figure 5-17. Final MSE Map using Sellmeier model and including the Bandwidth.

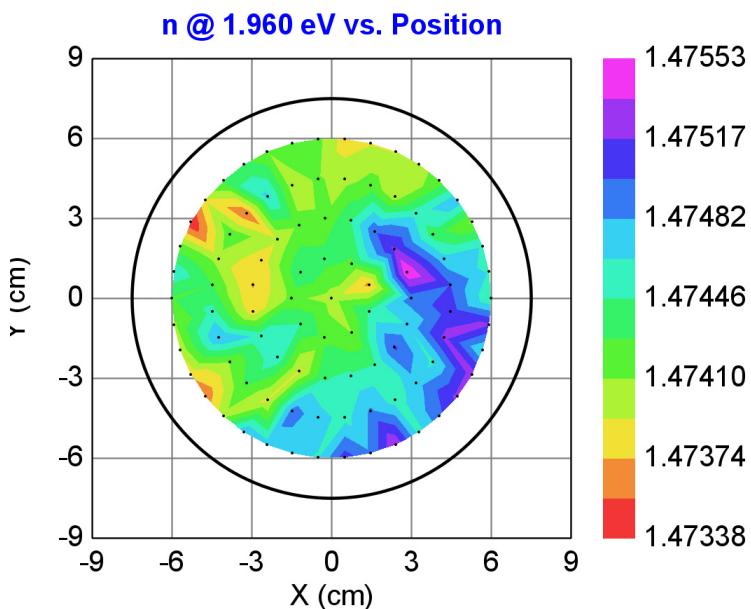


Figure 5-18. Final Index at 633nm (1.960eV) using Sellmeier model and including Bandwidth.

## 5.2. Multi-Sample Analysis

| FEATURES IN THIS EXAMPLE             |                              |
|--------------------------------------|------------------------------|
| • Selecting Multiple Points from Map | • Model: Multi-layer (empty) |
| • CTRL-SPACE BAR to switch views.    | • Select/Un-Select Data Set  |
| • Set Symbol Size                    | • Zoom on “Map”              |
| • Graph All Data Sets                | • Clear Multi-Data Set Mode  |
| • Multi-sample Analysis              | • Add Fit Parameter          |

Once again, we will be working with “mapped” data from multiple locations across a sample. This sample is more complex than the previous example. In addition to an SiO<sub>2</sub> coating across the wafer, there are 5 patterned locations on the substrate with an extra layer of Cr over the SiO<sub>2</sub> film. The Cr layers were deposited to nominally 10, 15, 20, 25, and 40nm thick. These layers are thin enough to allow light to penetrate through to the underlying SiO<sub>2</sub> film. They were part of a study of different ellipsometric methods to measure thin absorbing layers.<sup>3</sup> Figure 5-19 shows the location of each of the Cr regions, along with their nominal thicknesses in nanometers.

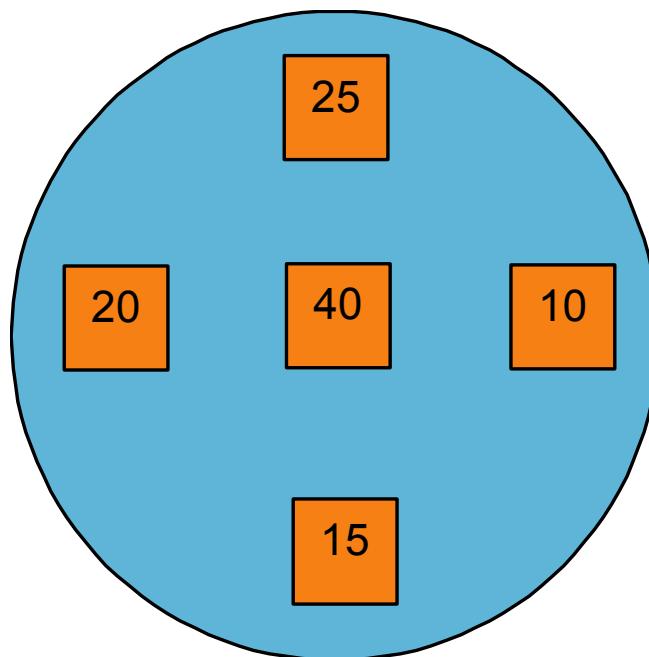


Figure 5-19. Overview of sample. The blue region represents a 100nm SiO<sub>2</sub> layer. At the five orange points, there is an additional Cr layer on the surface of the SiO<sub>2</sub> film, with the nominal thicknesses shown for each (in nm).

<sup>3</sup> J.N. Hilfiker et al. “Survey of methods to characterize thin absorbing films with Spectroscopic Ellipsometry”, *Thin Solid Films*, **516** (2008) pp. 7979-7989.

## Short-Cuts for Mapping Data

Before proceeding with this example, it is helpful to review the short-cuts when dealing with mapping data. The table below shows the important features we will use for this example.

Table 5-1. Short-cut reference for mapping data.

| SHORT CUT                     | FUNCTION   |
|-------------------------------|--|
| CTRL-Click on Point           | Select/De-Select Point                           |
| CTRL-ALT-Click on Point       | Delete Point                                     |
| CTRL-ALT-SHIFT Click on Point | Show camera image from point<br>(when available) |
| CTRL-SPACE Bar                | Switch view from single-point to Map             |

## Multi-Layer (empty) Model

Open the “Cr on SiO<sub>2</sub> MAP” data file. You will see the data from translation scan of the sample previously described – as shown in Figure 5-20. You can see “low” points in Psi at the 5 locations that have been coated with Cr. To fit this data, we need to first build a model. Because we need multiple layers, let’s try building the model from the very beginning. Open the “Multi-layer (empty)” model from the “Advanced” directory. This will appear as shown in Figure 5-21. Left-click on the Substrate = **none** and choose “Si\_Jaw” material file from the Semiconductor directory. Next, press the **Add** command and locate the next layer above the silicon substrate. For our first layer, choose a Cauchy – which we will use to model the SiO<sub>2</sub> layer. Turn on the “thickness”, “A”, “B”, and “C” Cauchy terms on as fit parameters. Next, go to the **+FIT Options** section and turn on the Thickness Prefit. This model should be adequate to fit any of the areas that do not have a Cr layer.

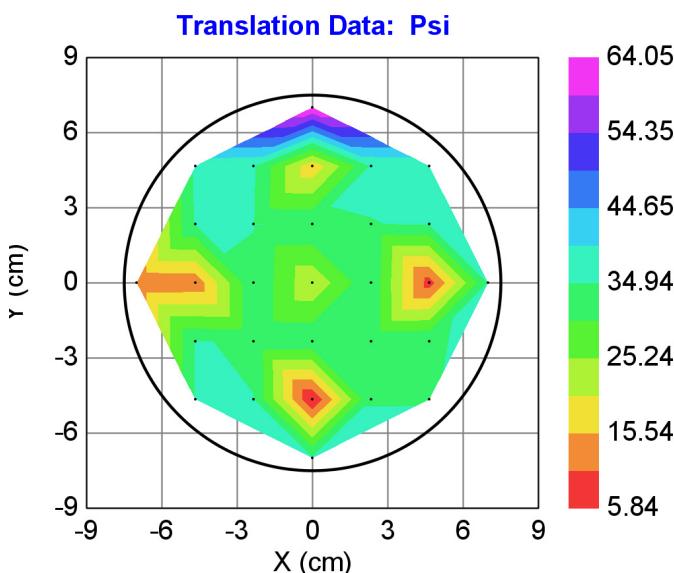


Figure 5-20. Translation scan graph for “Cr on SiO<sub>2</sub> MAP”.

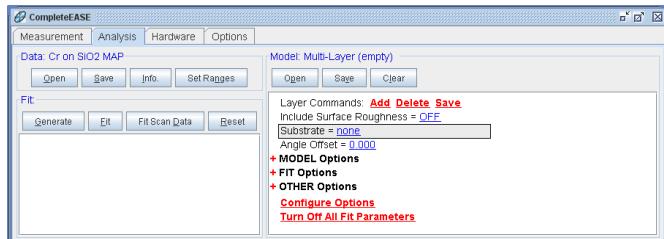


Figure 5-21. Starting with “Multi-layer (empty)” model.

## Set Symbol Size

Before continuing, let's increase the symbol size to better visualize the locations of the measured points. Right-click on the graph panel. If “Show Symbols” is not checked, do so at this time. From the right-click menu, choose “Set Symbol Size” as shown in Figure 5-22. Increase the symbol size from default value of 1 to 2 or 3. The graph shown in Figure 5-23 has symbol size set to “3”.

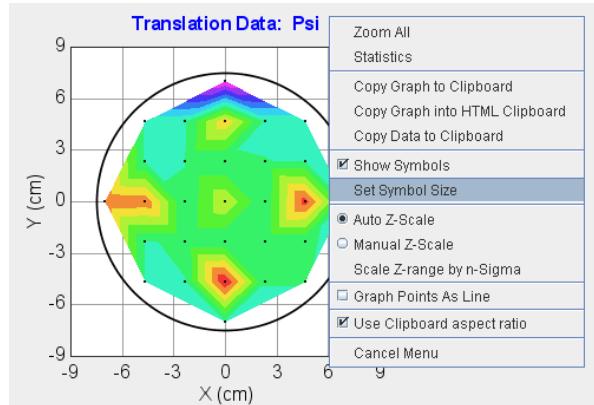


Figure 5-22. From right-click menu on graph, select the “Set Symbol Size” option.

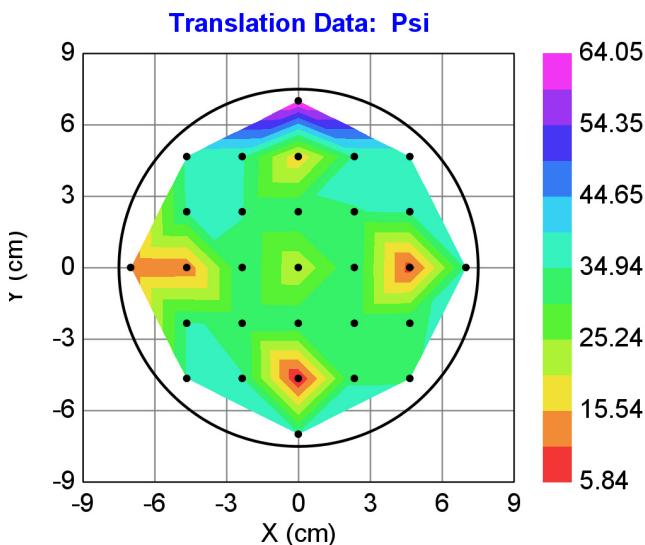


Figure 5-23. Figure with Symbol Size set to “3”.

## Zooming on Map

While this graph is not too complex, it is possible to collect hundreds or even thousands of points on the same sample. In these cases, it can be helpful to zoom into a certain location to better isolate a specific point. For demonstration purposes, drag your mouse across a region of the sample, as shown in Figure 5-24. The zoomed area is shown in Figure 5-25. To zoom back out to all points, simply right-click in the graph area and choose “Zoom All”.

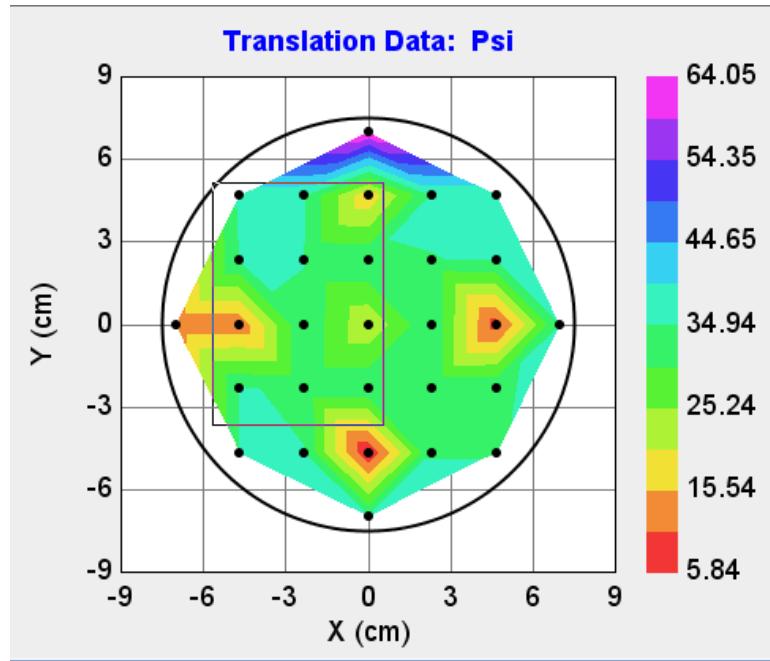


Figure 5-24. Drag your mouse over a graph area to zoom in to that region. A rectangle will show you the location of your “zoom” region.

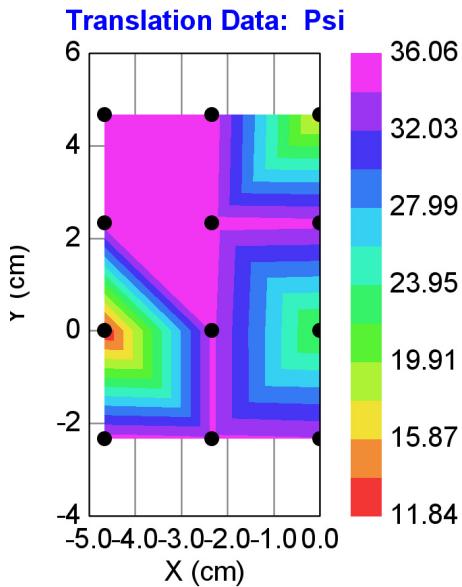


Figure 5-25. Zoomed-in area of the Map.

## Selecting Multiple Points on a Map

With our model ready to fit the  $\text{SiO}_2$  locations, go ahead and press your mouse on any of the points away from the Cr patterns (blue, purple, and dark green locations). The data from those locations will be opened and fit automatically, as shown in Figure 5-26. Next, go back to the map by checking “Show Map Data”. We are going to select data from multiple points – all of which only contain the  $\text{SiO}_2$  film – to be graphed and fit at the same time. To select multiple points, hold the CTRL button down when you press your mouse on the different areas. A larger grey circle will be shown around each data point that is selected, as shown in Figure 5-27.

The spectroscopic data for this example use eV for the wavelength default – a carry-over from the previous example.

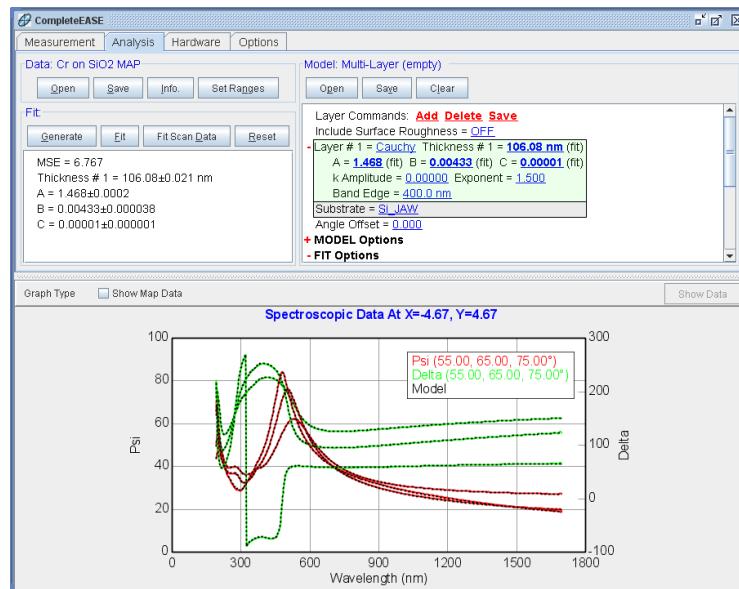


Figure 5-26. Cauchy fit to a single-point with only  $\text{SiO}_2$  film.

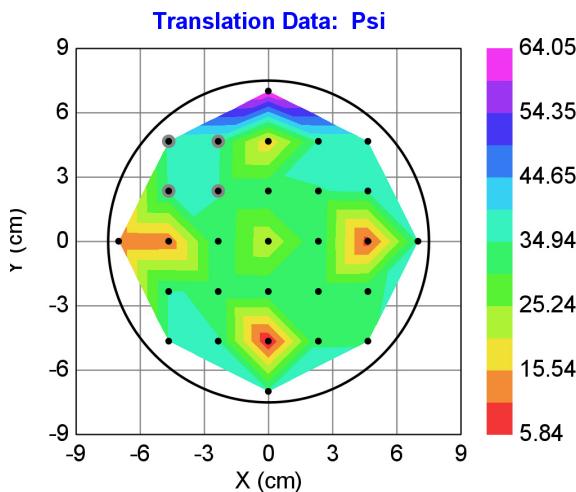


Figure 5-27. Graph with multiple points selected – as shown by the larger grey circle surrounding those points (4 pts in upper-left section).

## Changing the Graph

To toggle the graph from the “map” view of the graph to the individual spectroscopic data from a single point, you can either un-check the “Show Map Data” menu, or simply hold down the CTRL button and press the space bar. This also holds for returning to the “map” view. Try this a few times.

From the Spectroscopic View, we now have multiple points selected, so there is a new section to describe the location of each selected point and a check-box of whether all data should be graphed together or one-at-a-time. This is shown in Figure 5-28. Before, we had an MSE near 5 when fitting a single point. Press ‘Fit’ again and the MSE is now 22. That is because all 4 points are being fit to the same model and it can not match all points with a single answer (i.e. thickness needs to be different for each point).

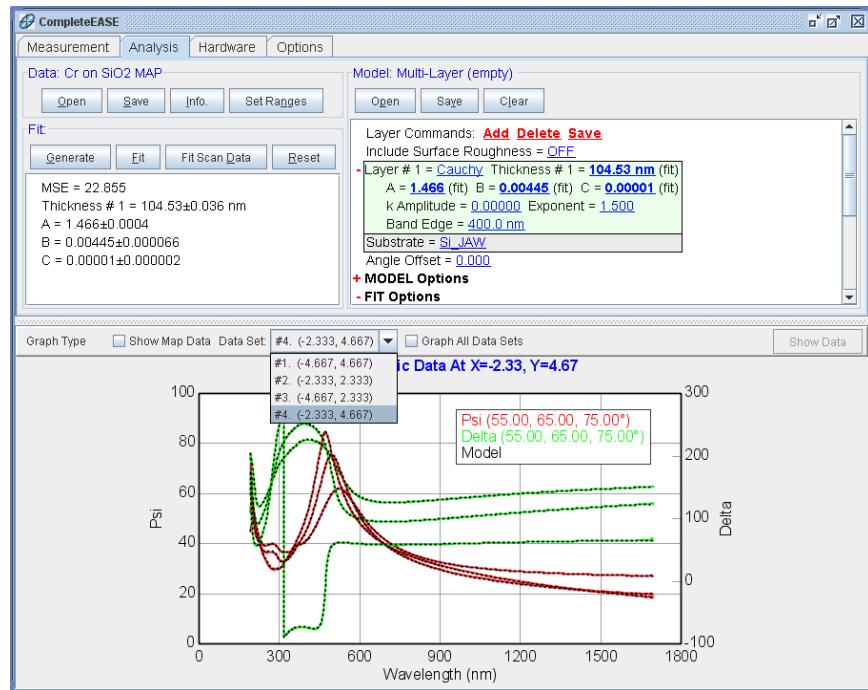


Figure 5-28. When multiple data points are selected, you can choose which point to view, or select the check-box to “Graph All Data Sets” simultaneously.

## Graph All Data Sets

There is slight variation between the four selected points. This is easier to visualize by graphing all data sets at the same time. Before proceeding, simplify the graph by turning off the double-Y axis and selecting only the 65 degree data (from ‘Set Ranges’ menu, as shown in Figure 5-29. Now, it is okay to check the “Graph All Data Sets” option and you see Psi curves from all four locations – see Figure 5-30.

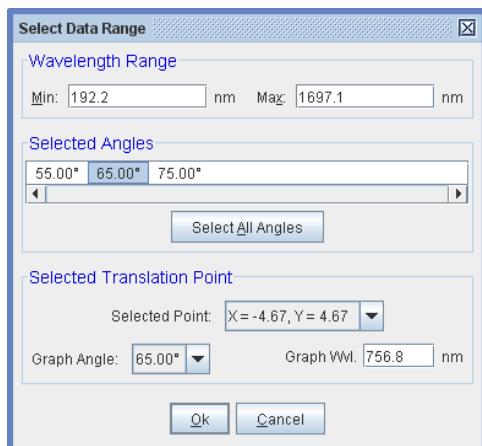


Figure 5-29. Choose ‘Set Ranges’ and select only the 65 degree data.

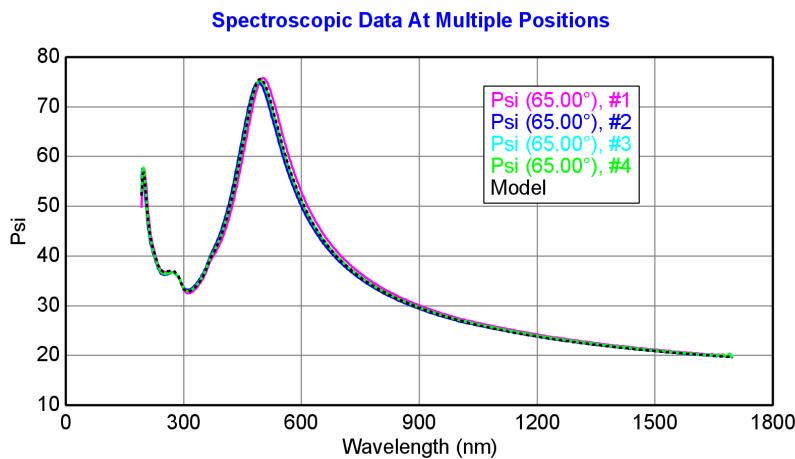


Figure 5-30. Graph of all four Psi curves from multiple data point selection.

## Selecting and Unselecting Data Sets

There is a right-click menu over the words “Data Set” above the graph that allow for selecting, unselecting, and clearing data sets. This menu is shown in Figure 5-31. A good test of these menus is to select each individual data set and fit the thickness for each point. If you only have a single data point selected, your MSE should be near six. Also, you can visualize which data set is selected by dropping down the list of data sets. Notice in Figure 5-32 that all points that are not selected are marked as such.



Figure 5-31. Right-click over the “Data Set” text above graph to get extra choices for selecting, unselecting, deleting, and clearing data sets.

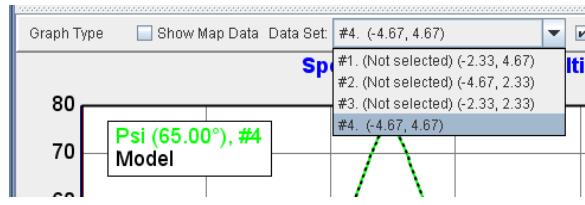


Figure 5-32. Drop-down list of points shows which are “(Not selected)”.

## Multi-sample Analysis

Thus far, we have fit each of the four selected points individually and as a combined group. However, when we fit them all together, we had a single set of fit parameters for the entire group. This may be okay for the Cauchy parameters – as the film is the same everywhere – but the thickness is NOT the same at each point. There is an advanced feature in CompleteEASE that allows multiple points to be fit simultaneously with some of the fit parameters common to all points and other fit parameters allowed to vary between points. Although the four points that are coated with SiO<sub>2</sub> do not benefit from this powerful technique, the demonstration for these points will help understand the basic concepts before applying to the Cr films – which can benefit from multi-sample analysis.

To use this method, first go to the bottom of the Model and choose **Configure Options**. Under the “Model Options” section, check “Multi-Sample Analysis” as an Available option. This is shown in Figure 5-33.

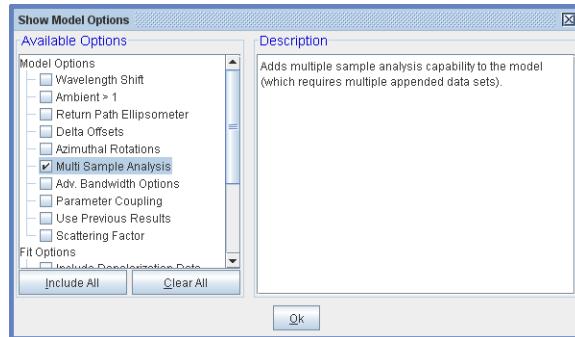


Figure 5-33. Check the “Multi-Sample Analysis” option from Model Options section.

Next, go to the +**Model Options** section and expand the newly available +**Multi-Sample Analysis** section. Press the [Add Fit Parameter](#) text and choose Thickness #1. The thickness for each “selected” data point will show up in the list below (as a fit parameter). Now, right-click on the “Data Set” text and choose to “Select ALL Data Sets”. This will allow us to vary and fit the thicknesses for all 4 locations in the Multi-sample analysis section. The Cauchy parameters will still be fit – but the same values will be used to fit all data sets simultaneously. Go ahead and press ‘Fit’. Figure 5-34 shows the final results after the multi-sample analysis. The graph shows the model matching each of the 4 curves – as four different thicknesses are fit along with a common set of Cauchy parameters.

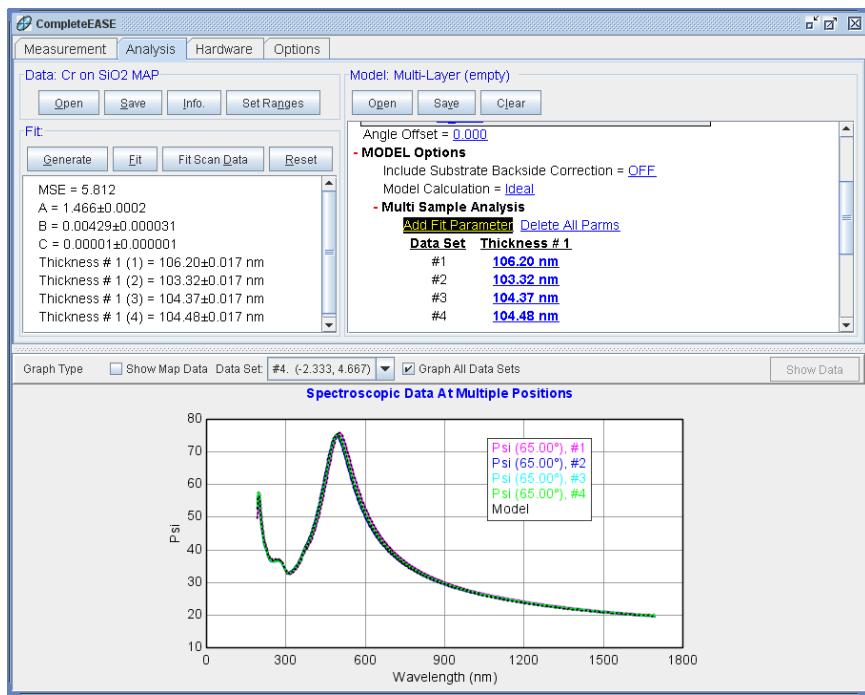


Figure 5-34. Fit results for multi-sample analysis of four locations of  $\text{SiO}_2$  on Si. A common set of Cauchy values is used, while the thickness of each  $\text{SiO}_2$  layer is allowed to vary in the **+Multi-Sample Analysis** section of the Model.

## Clear Multi-Data Set Mode

After the multi-sample analysis of four locations with  $\text{SiO}_2$ , the Cauchy values from the fit should be a good final result. We are now ready to turn our attention to the Cr coated areas. To remove the 4 locations with  $\text{SiO}_2$  only that are currently selected, press the “Data Sets” text above the graph with right-mouse button and choose “Clear Multi-Data Set Mode”. This returns to a single data set. Press CTRL-SPACE BAR to go back to the map view.

Before we proceed, we want to turn off the fit parameters for the  $\text{SiO}_2$  film – including the thickness and Cauchy values. We are going to select the Cr coated areas, but we don’t want the model to “automatically” try to fit this data – as we haven’t added a layer for the Cr film. To turn off the “auto” fitting mode, right-click your mouse in the **Fit** panel and un-select the “Auto Fit” option at top, as shown in Figure 5-35. Now, we can select a point without automatically fitting that point. Go ahead and select the point in direct center of graph (as shown in Figure 5-36).

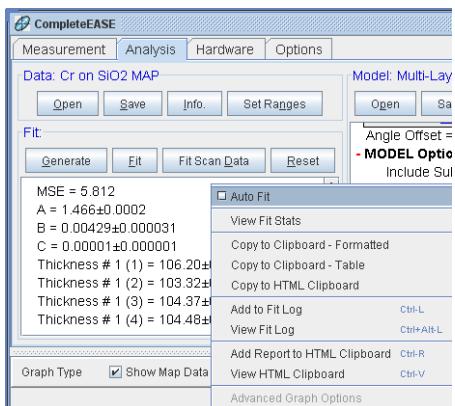


Figure 5-35. Right-click in the Fit panel and turn off the “Auto Fit” check-box.

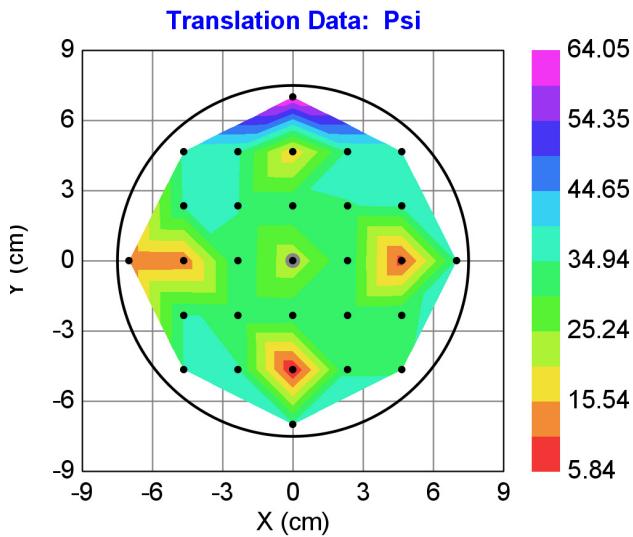


Figure 5-36. Select the center point of graph (shown surrounded by grey).

I show this data in Figure 5-37 with double-Y axis turned back on to show both Psi and Delta. I have also generated data to show how different the center-point data are compared to a model for the single-layer SiO<sub>2</sub> film.

Before fitting, we need to select ALL angles again.

To fit this data, we need to add another layer to our model. Press **Add** and choose location above SiO<sub>2</sub> film to add B-Spline layer from the Basic folder. Expand the B-Spline layer and press the Starting Mat = **none**. Choose Cr.mat from the Metal directory. This will calculate the B-Spline points to match Chromium optical constants as published in Palik’s Handbook of Optical Constants. Hold the SHIFT key and roll the mouse wheel over the thickness until it matches the data. Unfortunately, this film does not have the same optical constants as “book” values. This is common for metals, which will differ optically with different deposition methods and processing conditions. Roll the thickness to 40nm, which was the nominal thickness for the Cr layer at this location. The model with 40nm is compared to experimental data in Figure 5-38.

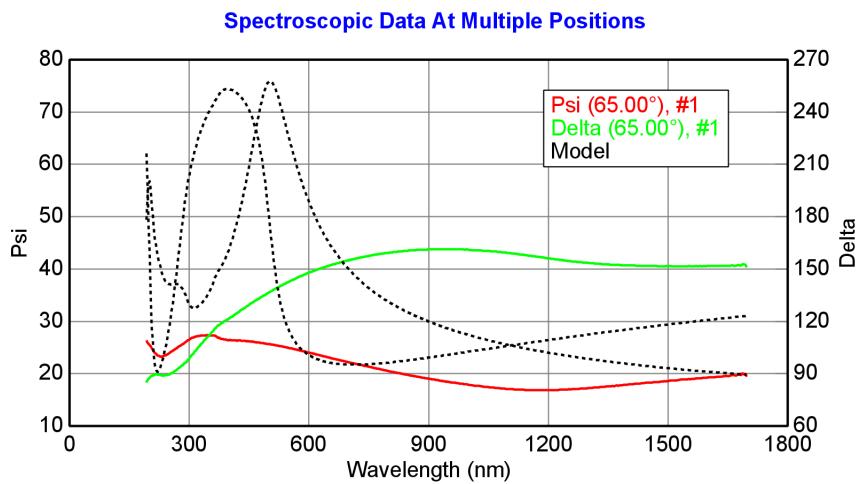


Figure 5-37. Data for center-point compared to model with single-layer  $\text{SiO}_2$ .

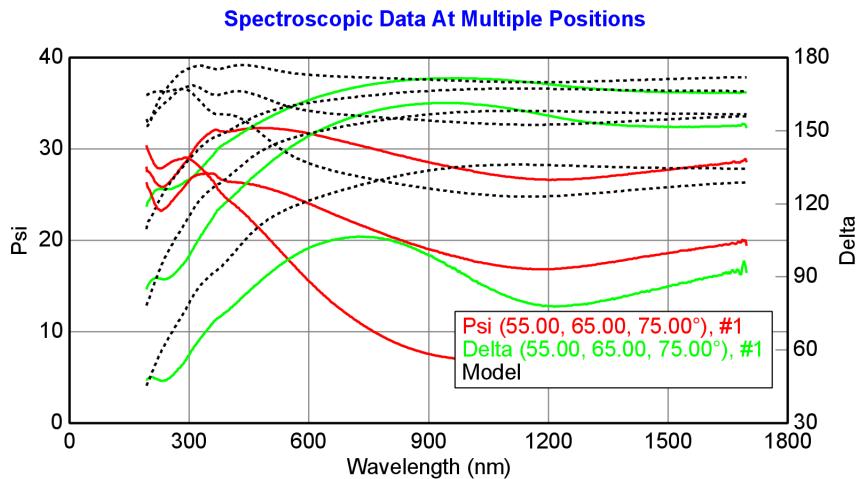


Figure 5-38. Model with 40nm of Cr (starting mat in B-Spline is Palik's Cr) compared to experimental data at center point.

Because the results are not very close, we need to either global fit the B-Spline parameters or fix the thickness to start. We will choose the latter, as we were given the nominal Cr thickness. With thickness FIXED at 40nm, go ahead and press ‘Fit’. The data fit reasonably well (see Figure 5-39), with an MSE around 4. However, there is a small bump in the model at 3.5eV that don’t match. This is an “interference enhancement” from underlying  $\text{SiO}_2$  film. We can only match this region with the correct Cr thickness. Now, turn on the Cr thickness and fit it as well. The final results appear as shown in Figure 5-40 with a good match across the spectrum and MSE near 2.

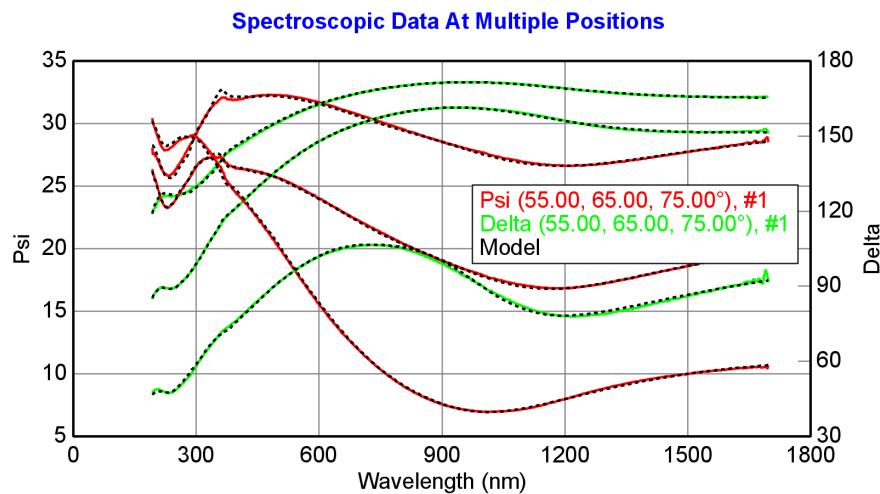


Figure 5-39. Fit to center point with 40nm fixed B-Spline thickness. The miss-match near 3.5eV is due to interference enhancement from the underlying SiO<sub>2</sub> film. The correct Cr thickness will match this region as well.

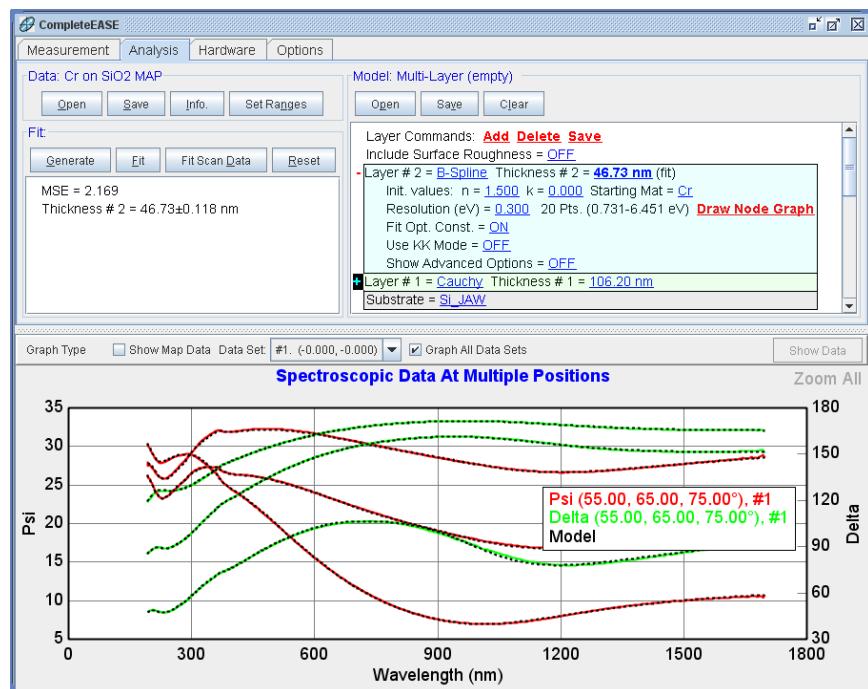


Figure 5-40. Final fit to center point.

## Multi-Sample Analysis (revisited)

Now that we have developed a model to match the center point – with Cr film on SiO<sub>2</sub> on Si – go ahead and try this model for all points that are coated with Cr. From the map view, press CTRL while choosing each point with the left mouse button. The points will appear with grey circles surrounding them, as shown in Figure 5-41.

Next, switch to the Spectroscopic View (CTRL-SPACE BAR) and turn off the double-Y axis and Set Ranges to only 65 degrees. This will allow a convenient comparison of the curves, as shown in Figure 5-42. From this data alone, we can estimate the points with thickest-to-thinnest Cr layers based on the shifts in data. The thickest point was at center (in purple). As the data shift, the Cr film gets thinner.

The order of points will differ depending on the order they were selected. Thus, your colors may not match the same order in our Figure.

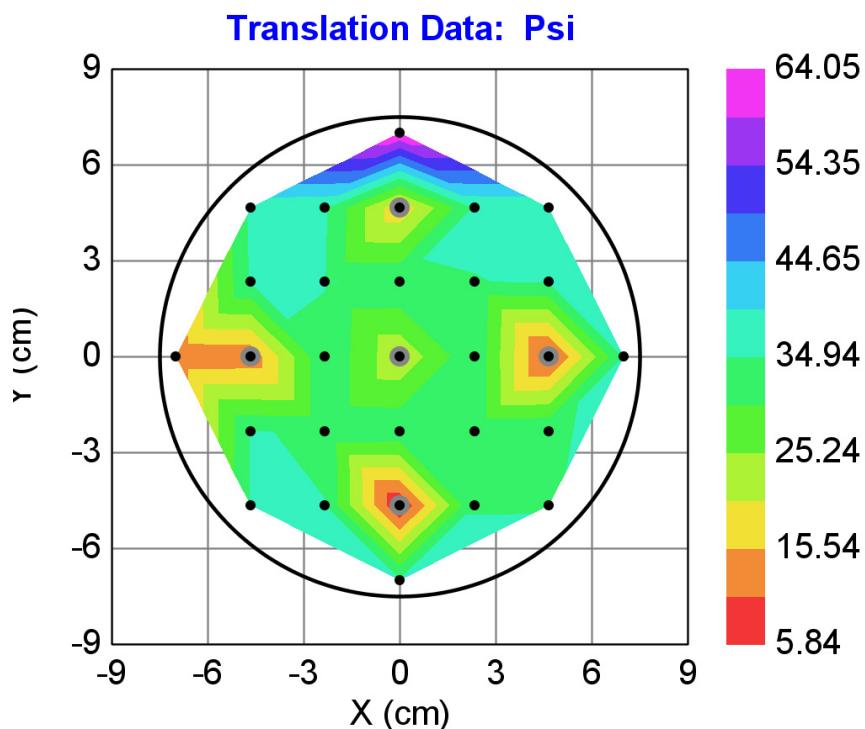


Figure 5-41. Map view with all 5 locations selected that have Cr coating over SiO<sub>2</sub>/Si.

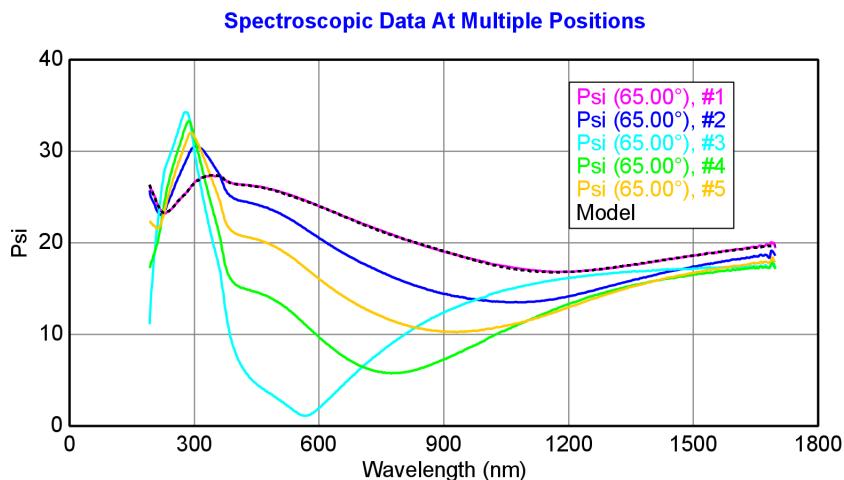


Figure 5-42. Spectroscopic Graph comparing the Psi curves from each of the 5 locations – with only 65 degree data selected.

Now, let's prepare the Multi-Sample Analysis. In the +MODEL Options section, you will see that the Thickness #1 parameter is still selected (Figure 5-43(a)). Press the Delete AllParms option to remove Thickness #1, as we will start with a common SiO<sub>2</sub> thickness and only allow the Cr thickness to vary. Next, press the Add Fit Parameter selection and choose Thickness #2 (Figure 5-43(b)).

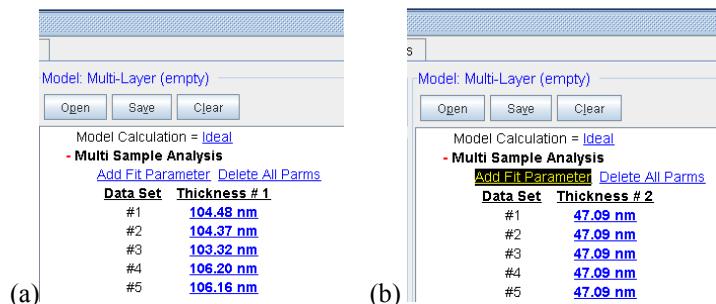


Figure 5-43. (a) Press [Delete AllParms](#) to remove the Thickness #1 parameter from the multi-sample analysis. (b) Next, press [Add Fit Parameter](#) and choose Thickness #2.

Before we begin fitting, we need to “tune” the different thickness values closer to their final result. For this purpose, un-check the “Graph All Data Sets”. Now, go down the list of points and SHIFT-Mouse Roll the different thicknesses shown under the Multi-Sample Analysis section until the Generated curve better matches the corresponding Experimental data curves. For more “fine” adjustment of the thickness, hold both the SHIFT-CTRL buttons and roll the mouse button. This decreases the thickness increment. An example is shown in Figure 5-44, where only Data Point #5 is selected and the 5<sup>th</sup> thickness is being rolled to better match the curves.

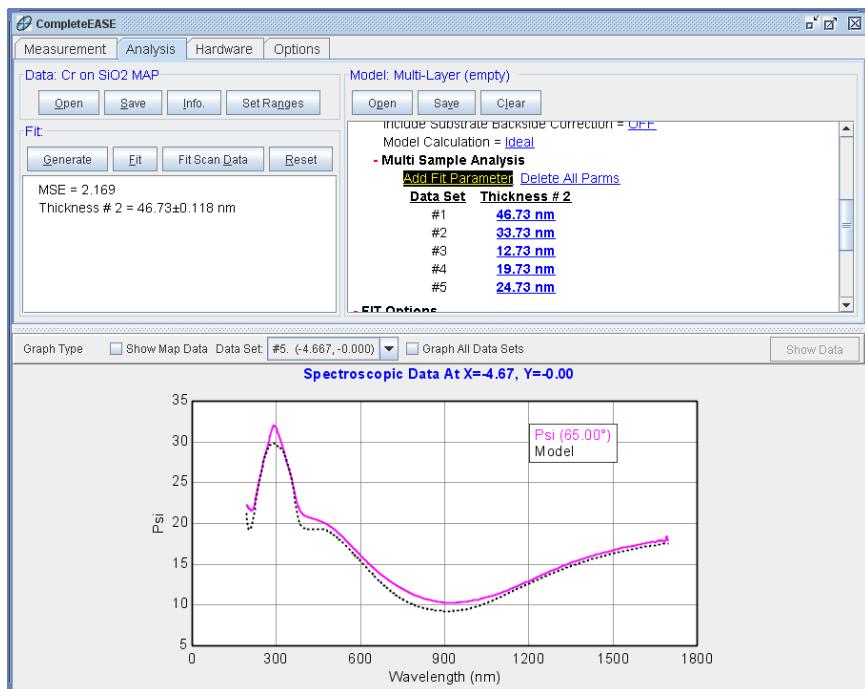


Figure 5-44. Match to Data Point 5 from rolling in the thickness under Multi-Sample Analysis section of the model.

After all data points have been matched individually, press the “Graph All Data Sets” menu again. Your graph should look similar to that in Figure 5-45. You hopefully noticed that the curves for thinner layers were not perfectly matched when we rolled the thickness. This is okay, as the thickest Cr layer does not match the optical constants for the thinner layers. In fact, we will later remove this point from the multi-sample analysis. For now, go ahead and press ‘Fit’. All five data points will be fit simultaneously with a single B-Spline layer to describe the common Cr optical constants and individual thicknesses for the Cr layers. The fit result should appear as shown in Figure 5-46. The MSE should be just under 20.

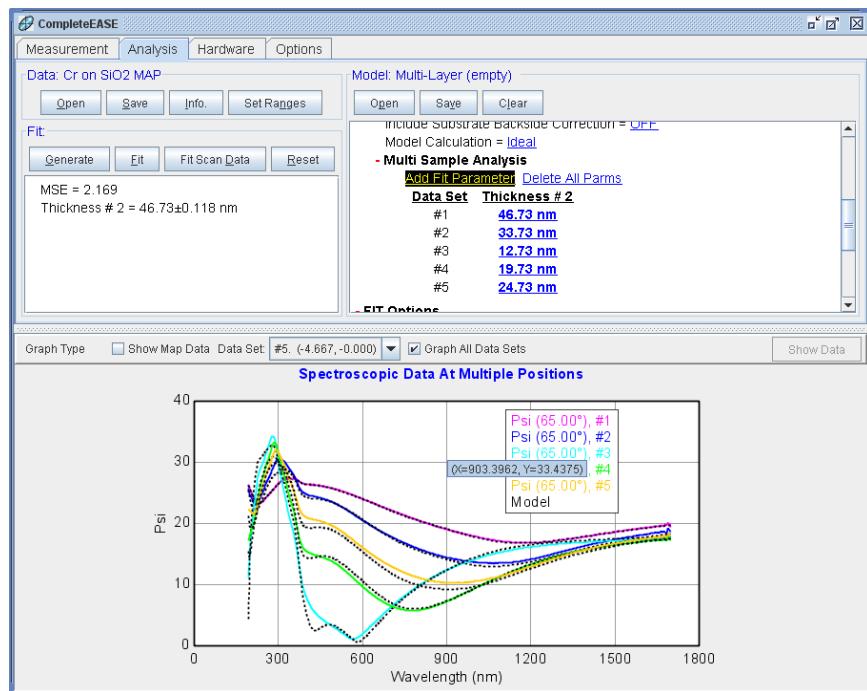


Figure 5-45. Preliminary data match by rolling individual thicknesses to pre-tune our guess to all 5 data sets before fitting multiple sample data.

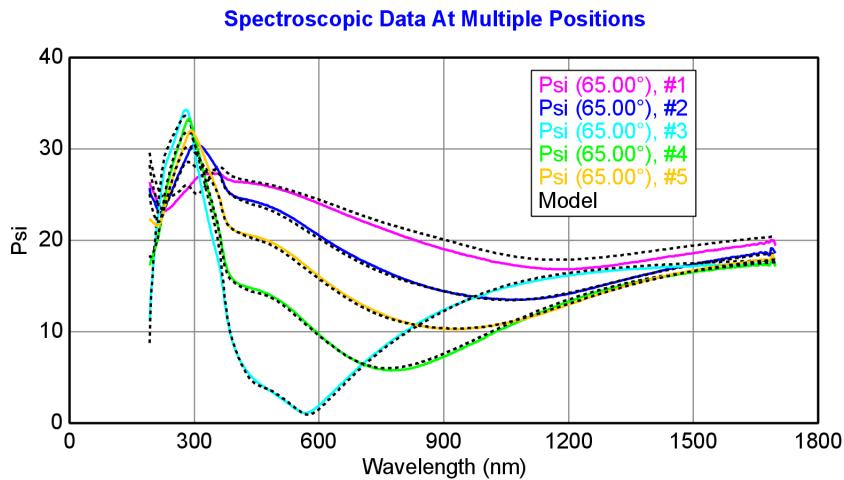


Figure 5-46. Fit result for all 5 locations with multi-sample analysis.

Now, let's remove the thickest layer from the multi-sample analysis. To do this, choose the Point location for the center point from the drop-down list above the graph. Next, right-click the mouse over "Data Set:" and choose to "Un-Select Data Set". The curve for the center point should disappear – leaving only four curves and their corresponding models. Press 'Fit' and the MSE should drop from above 19 to less than 14. The center (thickest Cr) point does not share the same optical constants as the thinner layers and thus is best left out of a multi-sample analysis. However, the problem is not confined to just the thickest layer. It turns out that the Cr layer optical constants appear to vary with thickness even for the thinner layers.

**NOTE:** The multi-sample analysis stayed intact by “un-selecting” the suspect center point. If instead we had deleted this point, the thicknesses listed in our multi-sample analysis would now be pointing to the wrong sample locations and we would need to roll these starting values over again.

Some of this variation is probably due to microstructure, possible roughness at the surface and oxidation. To test this theory, turn on surface roughness in the model and add it as another fit parameter in the Multi-Sample Analysis list. This will allow each point to have different amounts of roughness. Press ‘Fit’ and the MSE drops to near 9. The thickness of the rough surface increases with the thickness of the film (as shown in Figure 5-47). With this model, we could now add the thickest Cr point back into the model to see if this trend (increasing roughness) will better match the center point and be consistent (we expect larger roughness). Sure enough, the MSE for all five points drops below 12 with the results shown in Figure 5-48. At this point, research would continue by testing the samples with other techniques – such as Atomic Force Microscopy – to see if the roughness result is true for this sample.

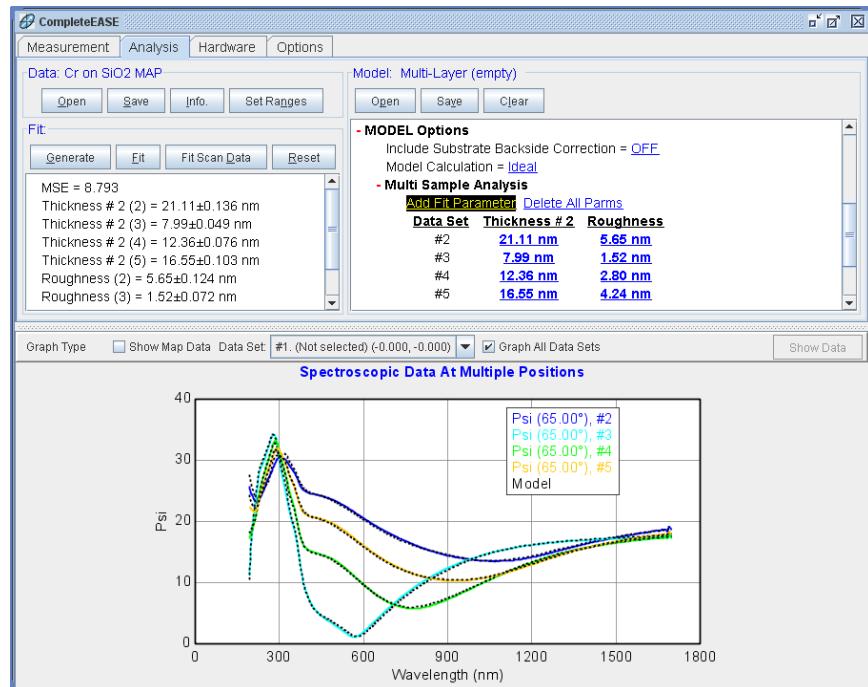


Figure 5-47. Fit to four thin Cr films with roughness added to the multi-sample analysis. Notice the resulting roughness increases as the Cr film thickness increases.

### - Multi Sample Analysis

[Add Fit Parameter](#) [Delete AllParms](#)

| Data Set | Thickness # 2            | Roughness               |
|----------|--------------------------|-------------------------|
| #1       | <a href="#">32.28 nm</a> | <a href="#">8.85 nm</a> |
| #2       | <a href="#">23.73 nm</a> | <a href="#">4.02 nm</a> |
| #3       | <a href="#">9.03 nm</a>  | <a href="#">1.10 nm</a> |
| #4       | <a href="#">13.92 nm</a> | <a href="#">1.97 nm</a> |
| #5       | <a href="#">18.61 nm</a> | <a href="#">3.02 nm</a> |

Figure 5-48. Fit results for all five points, showing increasing roughness with increasing Cr layer thickness.

As a final exercise press Data: > ‘Set Ranges’ and select all the angles back. Notice when multiple data sets are selected (with more than 1 angle), each data set is graphed with the same color. For example, all curves for Data #1 are in magenta and all curves for Data #2 are in blue. This helps to group them and reduce the total number of different colors graphed. Before fitting again, turn on the SiO<sub>2</sub> thickness as a fit parameter and add Thickness #1 to the list of Multi-Sample parameters. With all the angles selected and three different thicknesses included in the Multi-Sample Analysis, press ‘Fit’ and the results should appear as shown below. You will notice that the center SiO<sub>2</sub> thickness is larger than the remaining 4. However, this was verified on a separate wafer that was not coated with Cr. Thus, the larger SiO<sub>2</sub> thickness at center is to be expected. The final result is shown in Figure 5-49.

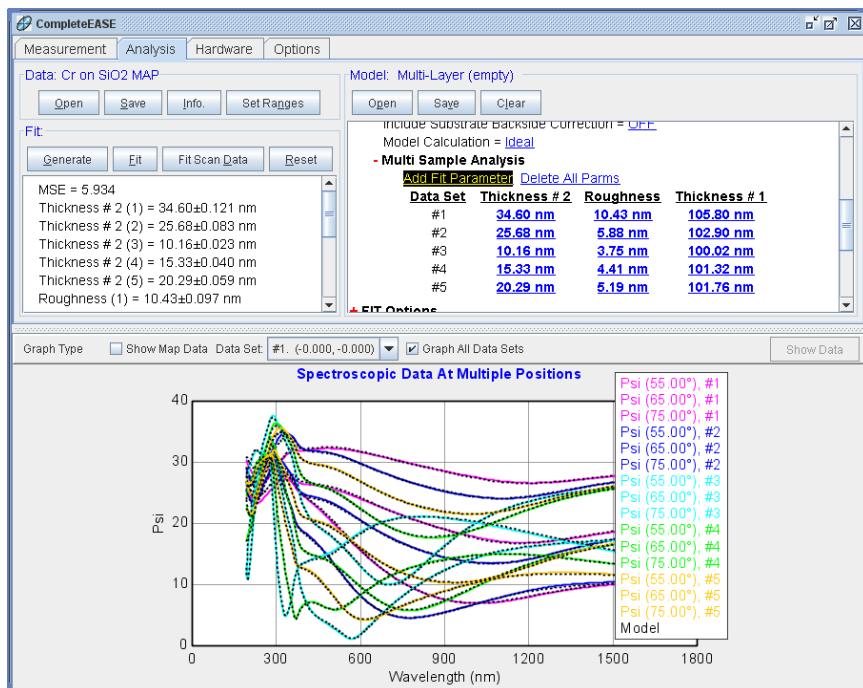


Figure 5-49. Final fit to all angles for 5 locations with Cr, SiO<sub>2</sub>, and Roughness thicknesses included in the multi-sample fit.

## 5.3. In Situ Data Analysis

| FEATURES IN THIS EXAMPLE   |   |
|--|---|
| • Viewing individual time-slices<br>• Selecting multiple-time slices from dynamic scan | • ‘Dynamic Fit’<br>• Multiple-Time Slice Analysis |

In Situ data provides ellipsometry measurements that were taken versus time. This often involves data as the thin films are being processed. The model may require a description of changes in film thickness, optical constants, composition, or even temperature versus time. The navigation, manipulation, and analysis of in situ data have many parallels with the corresponding processes for uniformity maps and multi-sample analysis. Thus, it can be helpful to review these examples before proceeding with this example.

This example is split into two sections. First, we will discuss navigating and selecting data sets from in situ time-dependent data set. These topics can be considered by any user-level. Second, we will work to analyze the in situ data via a multi-sample analysis approach and finally a time-dependent data analysis procedure. As this data comes from an amorphous silicon film and will require analysis methods including the B-Spline and Genosc layers, those examples should be reviewed in detail before proceeding with this example.

### Short-Cuts for Dynamic Data

Before proceeding with this example, it is helpful to review the short-cuts when dealing with in situ dynamic data. The table below shows the important features we will use for this example.

*Table 5-2. Short-cut reference for dynamic data.*

| SHORT CUT                | FUNCTION  |
|--------------------------|---|
| Click on Dynamic Graph   | Opens Spectroscopic Data from that time point.  |
| CTRL-Click Dynamic Graph | Selects Spectroscopic Data from that time point.<br>(Repeat for multiple time selections) |
| CTRL-SPACE Bar           | Switch view from dynamic to spectroscopic data.   |

## Navigating In Situ Data

Open “a-Si Grow Sim.iSE” data file from Examples folder. The time dependent data will be shown in the graph in Figure 5-50. Notice a selection of 5 wavelengths is graphed. These curves are not the only wavelengths measured, but represent the shape versus time for the spectral range selected.

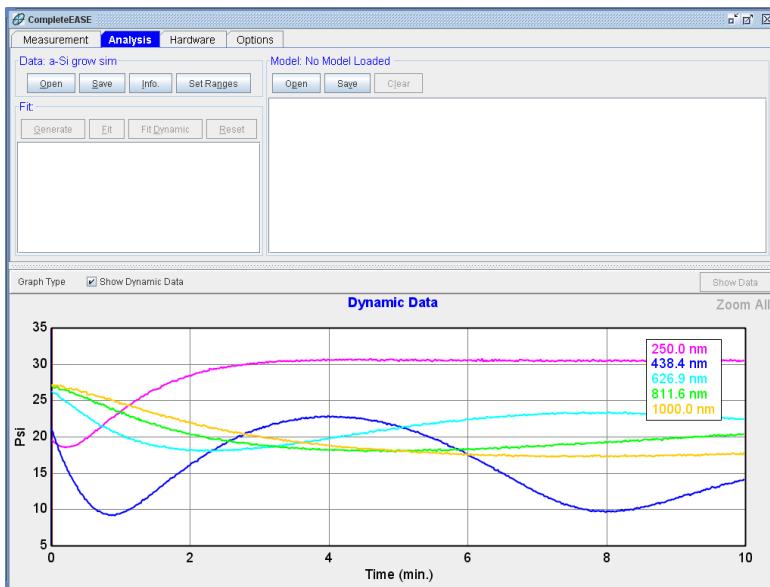


Figure 5-50. Graph shows in situ data versus time.

## Viewing Spectroscopic Data at a Specific Time

Left-click your mouse to select data for a specific time-slice. A line is drawn at that time slice, as show in Figure 5-51. Now, you can either press CTRL-SPACE BAR to toggle to the spectroscopic graph for that time-slice or “un-check” the box named Show Dynamic Data located just above the graph. Data for a time-slice selected near 3 minutes is shown in Figure 5-52.

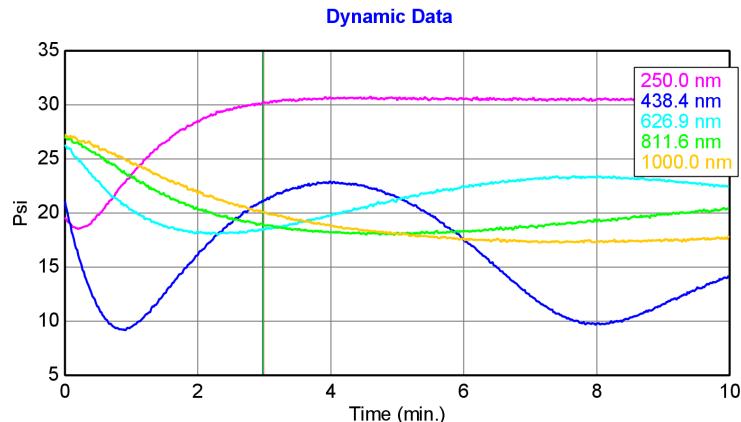


Figure 5-51. Left-click mouse on graph near 3 minutes selects this time and shows the selection as a vertical gray bar.

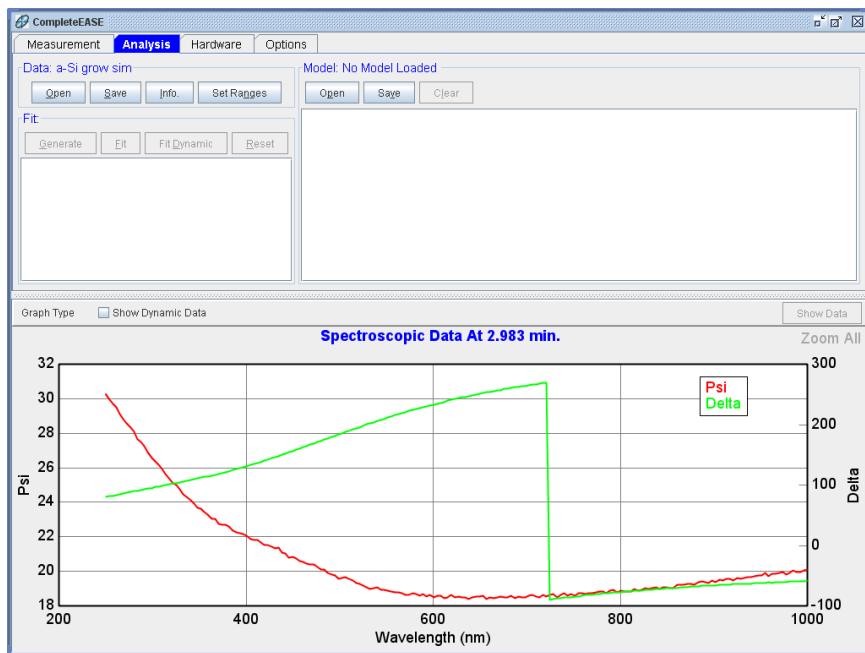


Figure 5-52. To view the spectroscopic data at the selected time-slice, press “CTRL-SPACE BAR” or un-check the Show Dynamic Data button just above the graph panel.

## Turning off the “Auto-Fit” function

Now, let’s build a model to fit this time-slice. You should be able to do this step with any time-slice between 2 and 3 minutes. Before we proceed, you will want to turn off the “Auto-Fit” function so the data are not automatically fit every-time we select a time slice or open a new model. To do this, right-click in the Fit panel region and un-check the Auto Fit option, as shown in Figure 5-53.

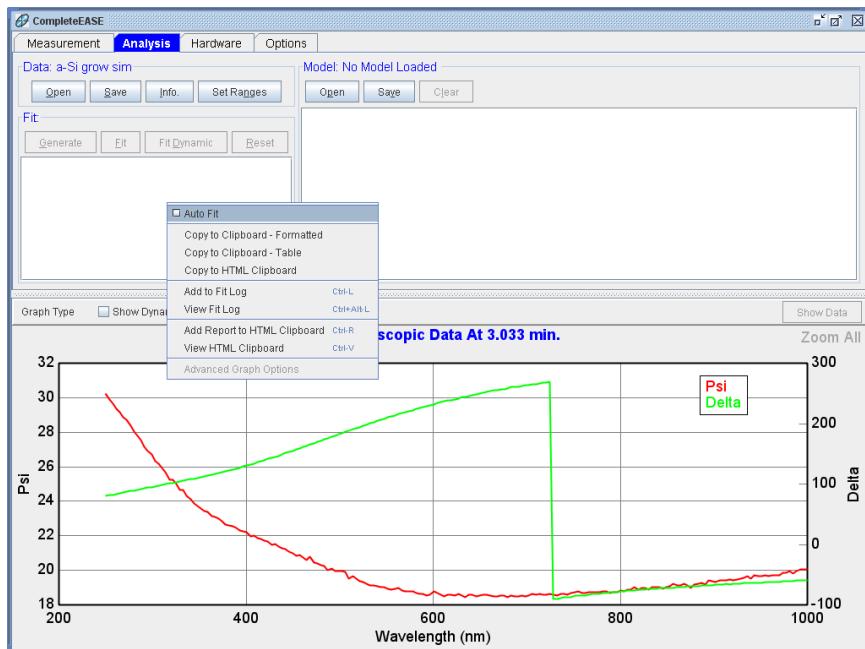


Figure 5-53. Right-click in the Fit panel region and turn off the “Auto-Fit” check-box.

## Building a Model

We will start with the assumption that we measure a coating that has known optical constants. This will allow us a model and find the thickness at any point in time. For our model, start with “BK7 Glass” substrate from the Dielectrics subdirectory and then add “a-si parameterized” from the Semiconductor directory. Start by fitting the a-si parameterized layer thickness only. You will find the fit is not adequate, as shown in Figure 5-54.

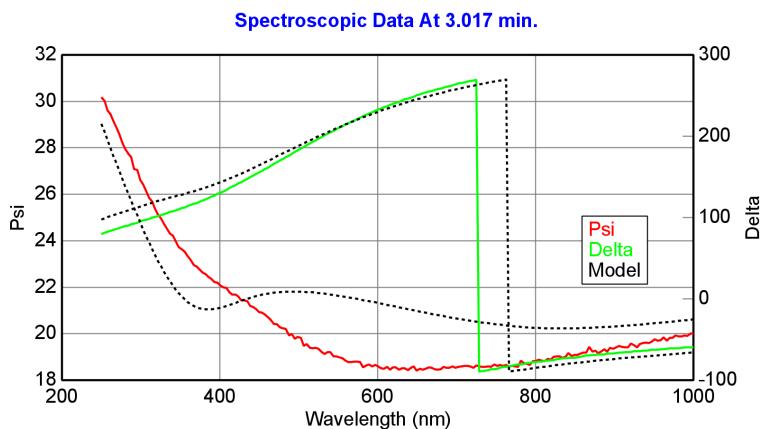


Figure 5-54. Fit result for data near 3 minutes when only fitting the a-Si layer thickness (no surface layer).

To improve the fit, we must consider that the surface of any silicon layer will be oxidized and possibly rough. To fit the surface, we can either add an SiO<sub>2</sub> layer or simply turn on the surface roughness thickness as a fit parameter. The improved fit result is shown in Figure 5-55.

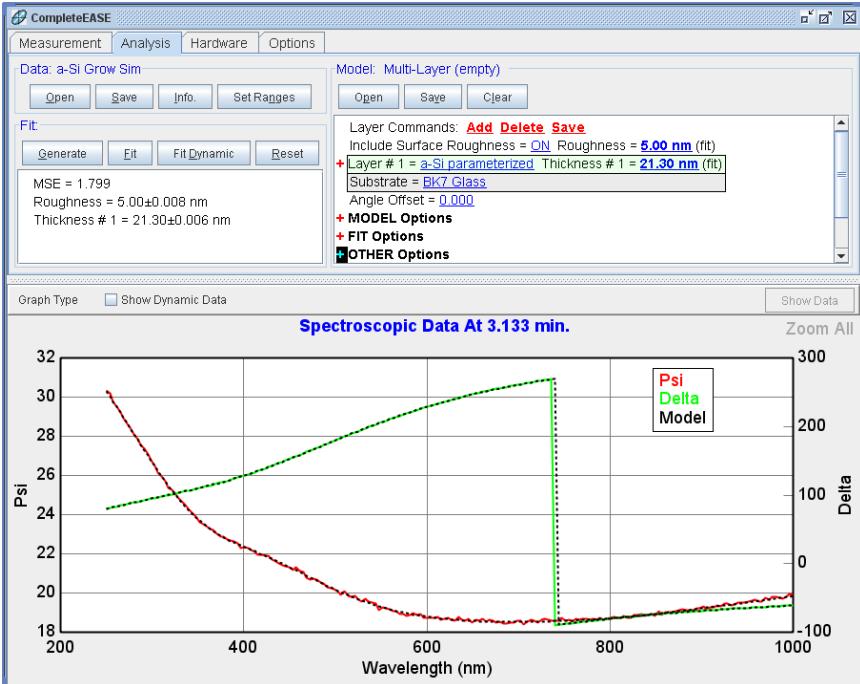


Figure 5-55. Fit result for time near 3 minutes when including the surface roughness.

## 'Fit Dynamic'

Now, let's fit these two parameters versus time to see how they change as the data vary across the measured time span. Simply click the Fit Dynamic button in the Fit panel and the software will progress from the earliest time slice and fit the data, continuing toward larger times, as shown in Figure 5-56.

You may notice problems starting a dynamic fit with model that is tuned for a thicker region of the data. If the fit fails, it may appear as shown in Figure 5-57. Here, the fit finally matches the data at around 3 minutes. To solve this problem, simply "tune" the fit for an earlier time before pressing Dynamic Fit. Go ahead and select a time slice near 0.3 minutes. Roll the thickness values for the roughness and a-Si layer until they are closer to correct for this new time. Press Fit for the single-point and you should get a result like shown in Figure 5-58. Now, press "Dynamic Fit" again and this time it should be successful. Press "Show Dynamic Data" to ensure the model curves match the Experimental curves over all times, as shown in Figure 5-59.

**NOTE:** It can be beneficial for many applications to start the fit from end-point rather than starting time, as the film thickness is often larger at the end of a data run. To fit the data in reverse-time order, right-click the 'Fit Dynamic' button and select "Fit Backwards in Time".

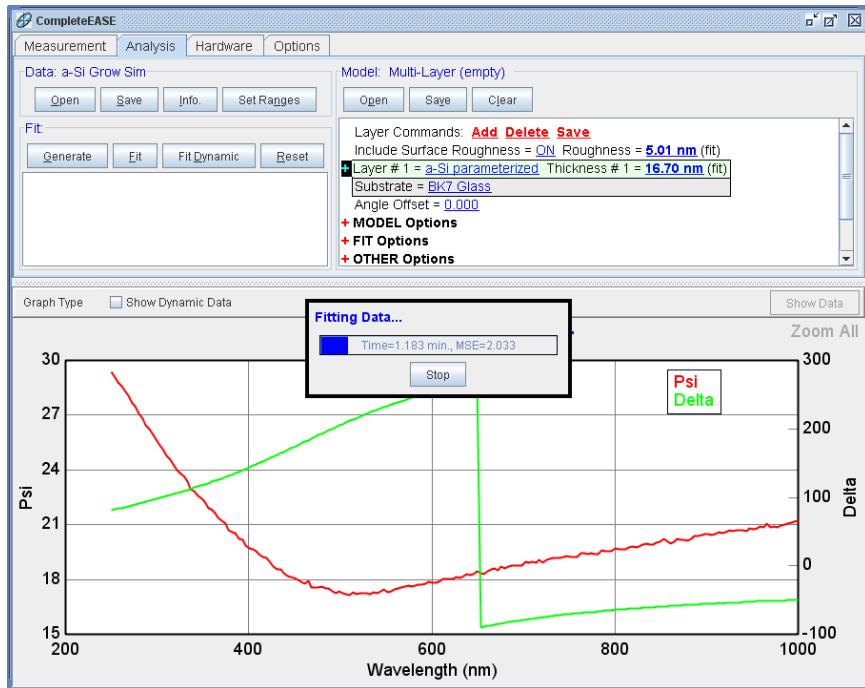


Figure 5-56. Data during Dynamic Fit of all measurement times.

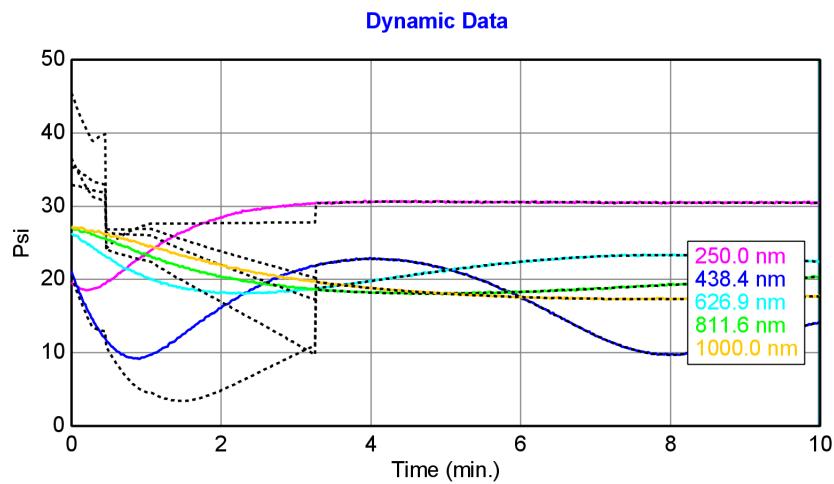


Figure 5-57. Fit fails until about 3 minutes because the starting thickness was not close for early time region.

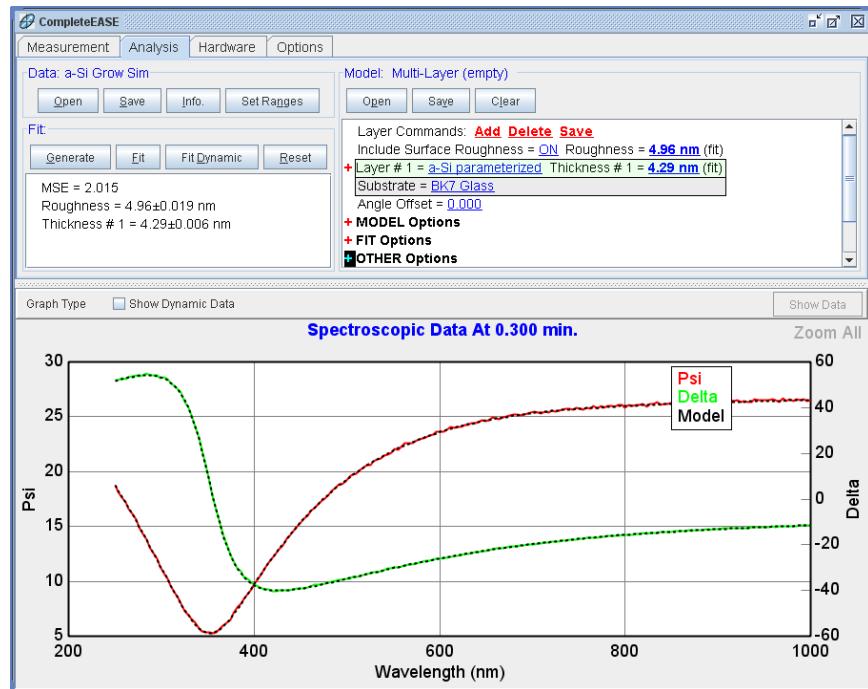


Figure 5-58. Fit for a-Si and rough layer thickness at time slice near 0.3 minutes.

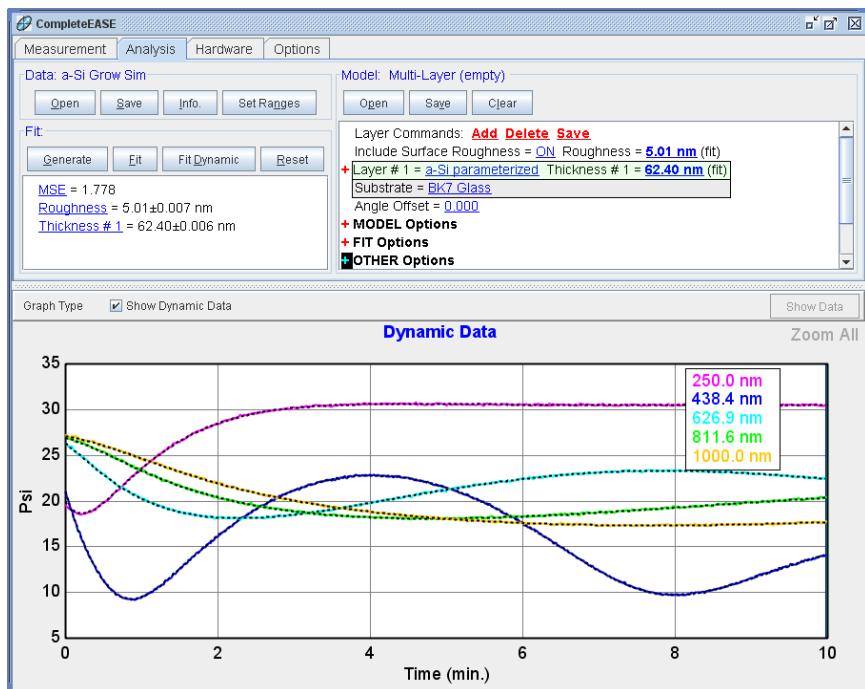


Figure 5-59. Result for Dynamic Fit when it is successful.

You will also notice in Figure 5-59 that the Fit Panel shows the final results (from last time). If you select the MSE, Roughness, or Thickness #1 with your mouse, the time-dependence of these values will be graphed, as demonstrated in Figure 5-60 and Figure 5-61.

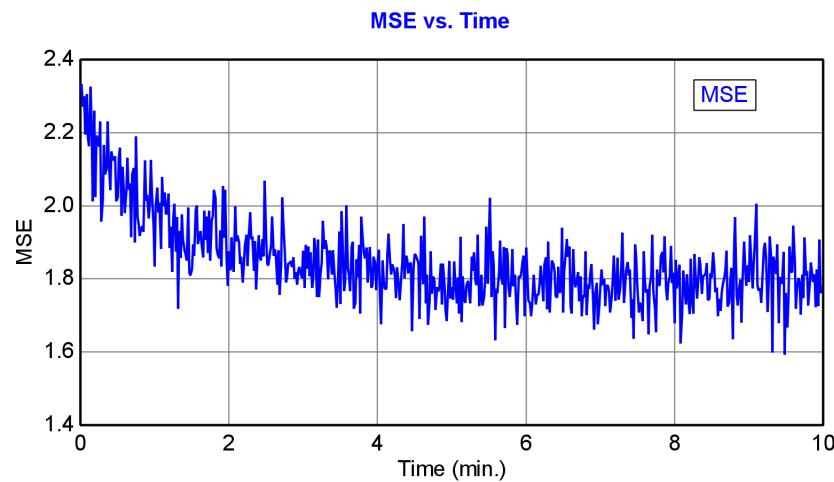


Figure 5-60. MSE values versus time after Dynamic Fit.

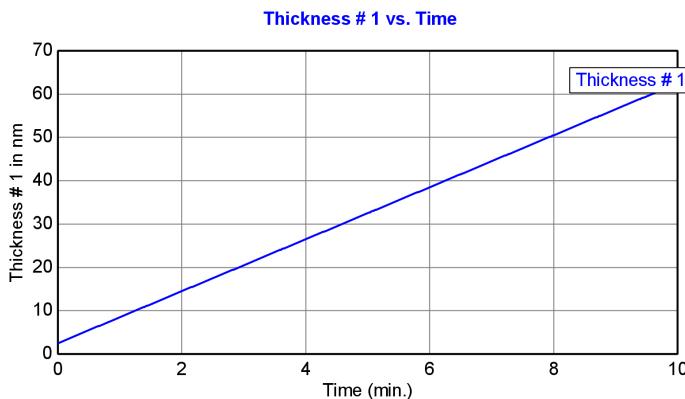


Figure 5-61. Thickness values versus time after Dynamic Fit.

## Selecting Multiple Time-Slices

For many materials, the optical constants will not be known and in situ data can be very effective to determine thickness and optical constants. The main advantage of in situ data is that it provides information about the sample at different stages of growth. If multiple time-slices are fit simultaneously, we get the same advantages as with multi-sample analysis (see section). To setup a multi-time slice analysis, view the Dynamic Scan Data and then hold the CTRL key down when selecting the multiple positions with your left-mouse button. An example is shown in Figure 5-62. These can now be viewed simultaneously in a similar manner as shown for mapping data. Un-check the “Show Dynamic Data” box and then you can choose which time slice you would like to view from a drop-down box. You can also view all data sets simultaneously by checking the “Graph All Data Sets” box, as shown in Figure 5-63 (here I have also turned off the double-Y axis on graph for simplicity).

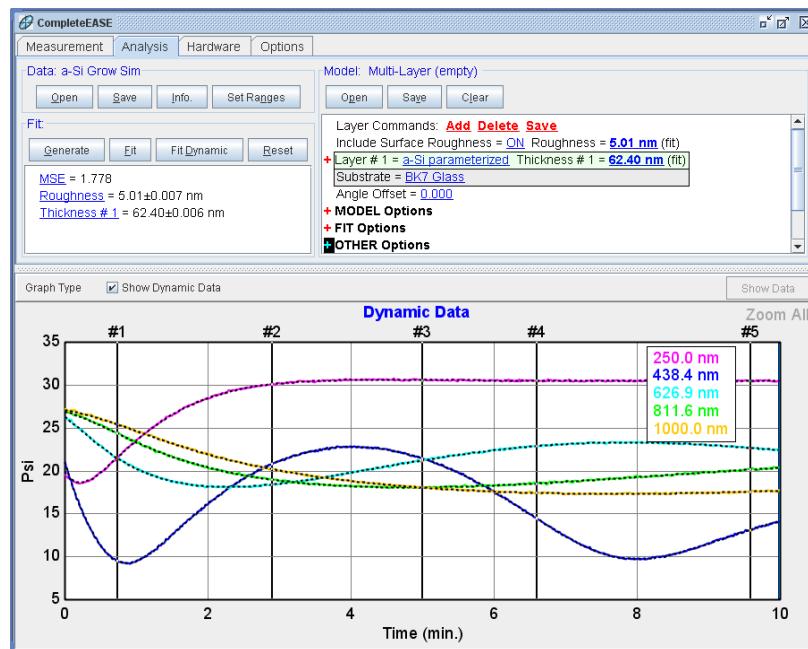


Figure 5-62. Holding CTRL button while left-clicking mouse on graph allows multiple time-slices to be selected.

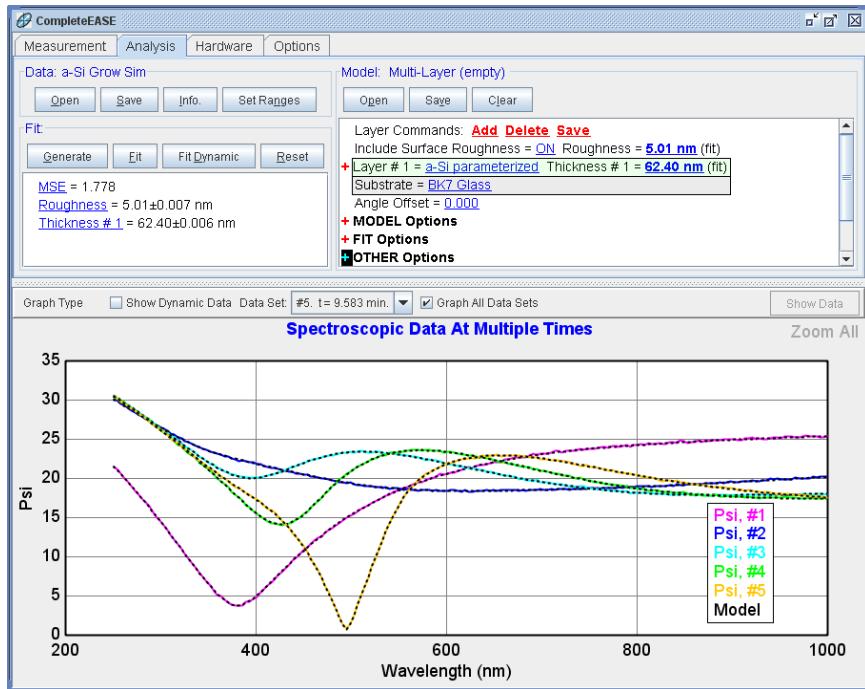


Figure 5-63. Graphing spectroscopic data from multiple time-slices.

## Manipulating Multi-Data Sets

Just like when manipulating multiple data sets from a “map”, there are additional options by right-clicking over the words “Data Set” just above the graph, as shown in Figure 5-64. For example, this is where we would go to “Clear Multi-Data Set Mode”.

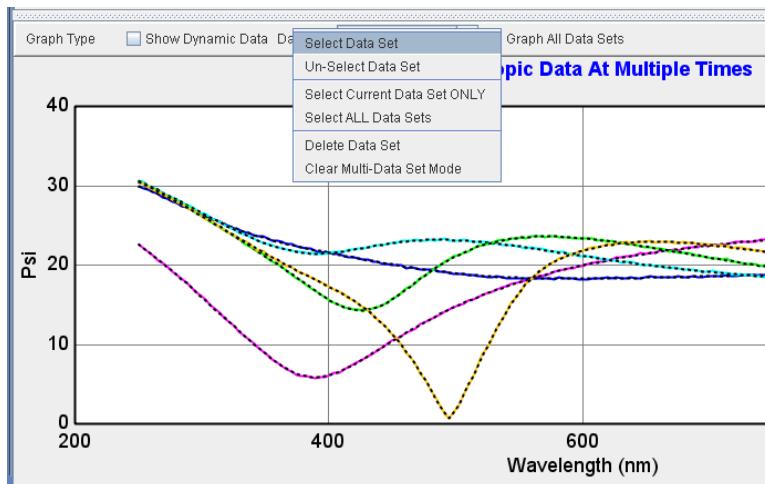


Figure 5-64. Right-click on the words “Data Set” above a graph to access additional options related to the multiple time-slice data sets.

## Multi-Time Slice Analysis

Now, let's setup the multiple time-slice analysis. From the Model panel, press the Configure Options menu at the bottom and then select "Multi Sample Analysis" from the choices of Available Model Options, as shown in Figure 5-65. This is a hidden feature as it is reserved for advanced users. Now, when we expand the Model Options section, there is a Multiple Sample Analysis section that can be further expanded. Click to "Add Fit Parameter" within this section and you will be able to define any of the fit parameters as variable for different time-slices. Let's do this for Thickness #1, as shown in Figure 5-66. It will seed the current thickness for all time-slices. This will not be correct and it is important to individually adjust the thickness "starting-points" for each time slice. This can be done by selecting each time slice individually in the graph and then rolling the thickness of the corresponding time-slice from within the Multi-Sample Analysis section, as I have done in Figure 5-67.

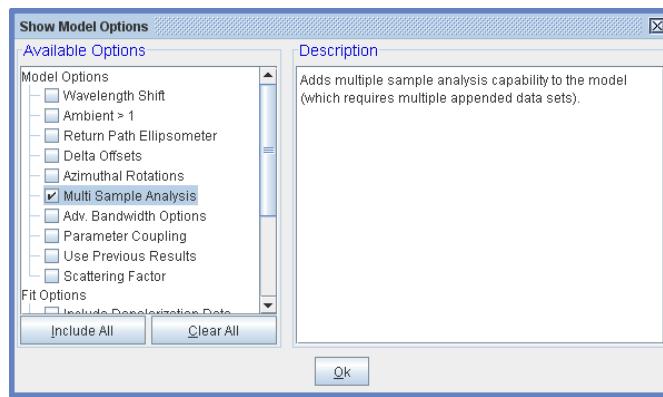


Figure 5-65. Choose "Multi Sample Analysis" from the Available Model Options within the Configure Options selection.

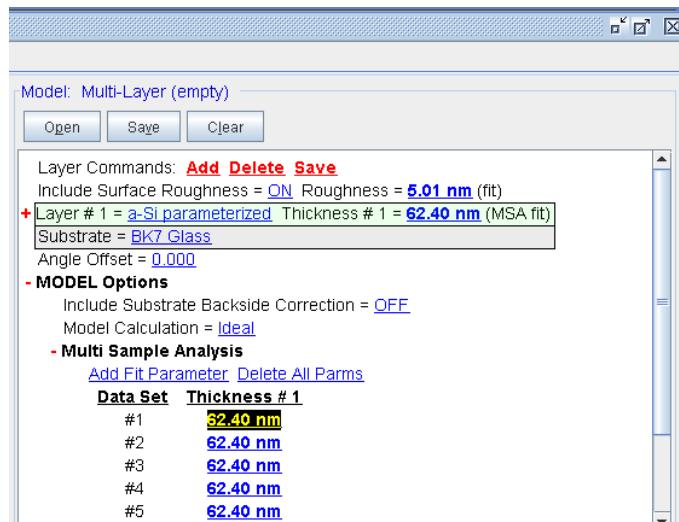


Figure 5-66. Model Options section is expanded to view the newly added Multi Sample Analysis section. Press "Add Fit Parameter" to designate a fit parameter to vary with each time-slice.

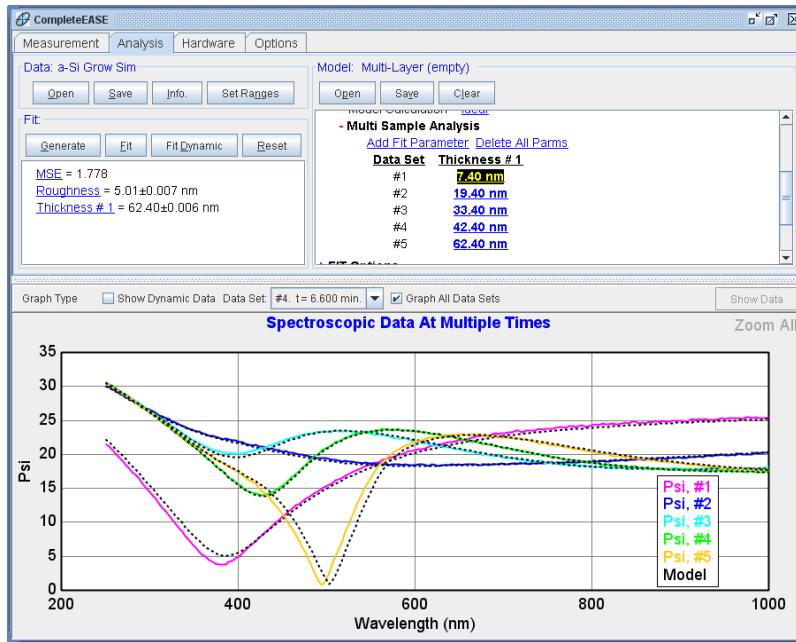


Figure 5-67. Starting points for all time-slices have been adjusted by rolling the mouse over each individual thickness from within the multi-sample analysis section of the Model.

You can now press ‘Fit’ and all thicknesses (for each time slice) along with a single roughness value that is used to fit all data sets is varied. This result is shown in Figure 5-68. If the roughness was also changing with time, its thickness could be added as a time-dependent variable within the multi-sample analysis section.

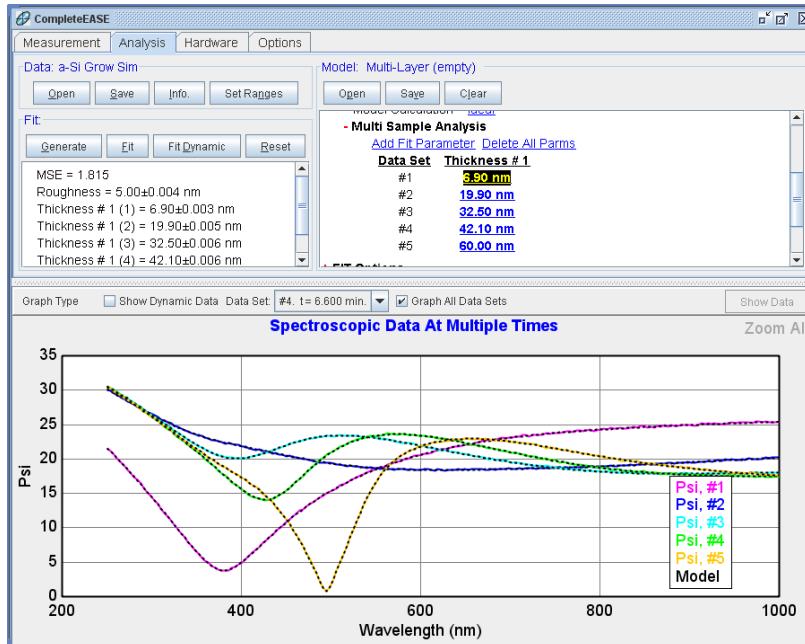


Figure 5-68. Fit results when a-Si thicknesses were allowed to vary at each of the five time-slices, along with a single roughness for all time slices.

## Fitting Optical Constants

The real benefit of multi-time slice analysis is that it allows better results when fitting optical constants for a layer. Let's pretend we don't know the optical constants for this amorphous silicon layer. Replace the coating in your model with a B-Spline layer. To get the B-Spline optical constants in the general vicinity of the final answer, we will click on the "Starting Mat =" and choose a-Si from the Semiconductor directory. This will seed the node values of the B-Spline to match the reference a-Si optical constants, as shown in Figure 5-69.

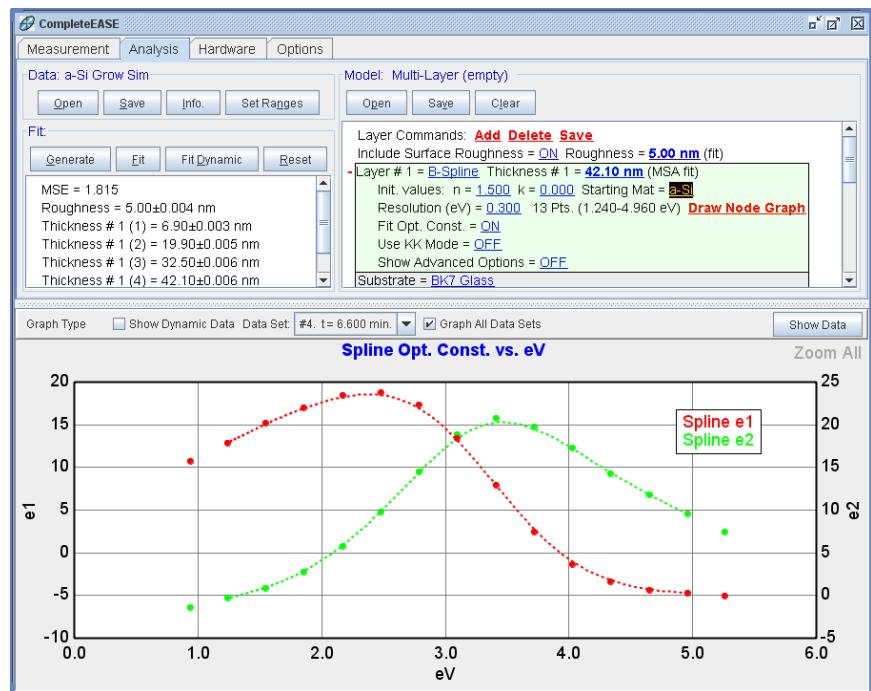
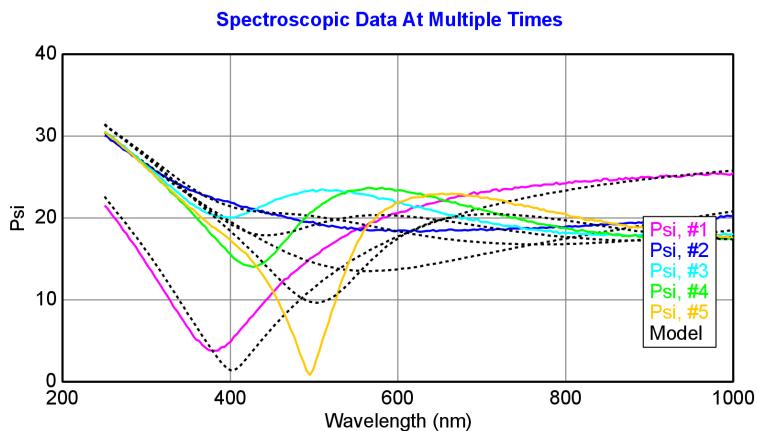
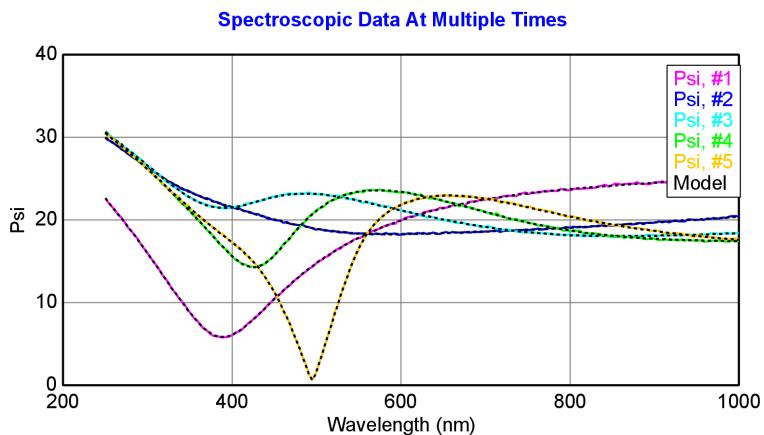


Figure 5-69. Starting with a B-Spline layer, choose "a-Si" for the Starting Mat to get the node values in the correct general shape for this type of film.

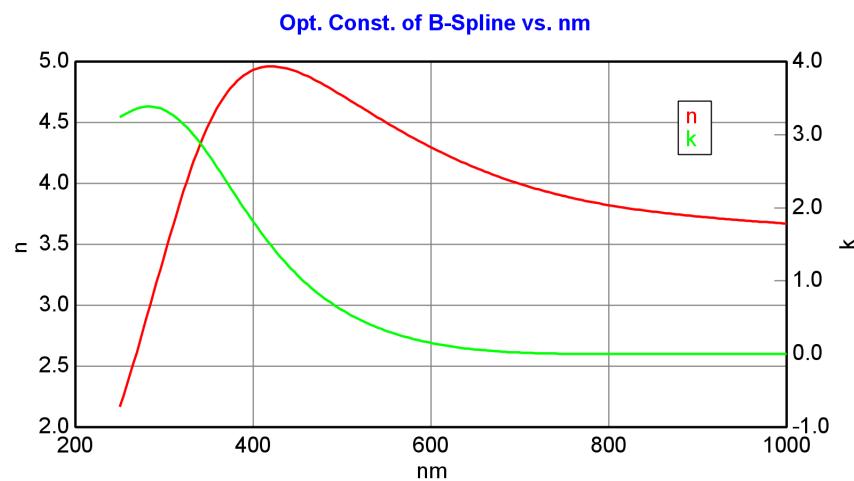
You will notice that the starting point is not the correct final optical constants for the time-dependent silicon simply by Generating data, as shown in Figure 5-70. However, we have five time slices to provide adequate information about this film at different thicknesses. Go ahead and press 'Fit'. The node values will adjust in the B-Spline to best fit the amorphous silicon data from ALL time-slices simultaneously. This fit result is shown in Figure 5-71, with the B-Spline optical constants shown in Figure 5-72.



*Figure 5-70. Generate Data and you see that the book-value a-Si optical constants used as a starting point in our B-Spline do not match the experimental data. However, they are close enough to give us a good starting point for fitting.*



*Figure 5-71. Fit results with B-Spline Optical constants allowed to vary.*



*Figure 5-72. Final optical constants from B-Spline fit.*

## 5.4. Creating OC Library for Composition or Temperature-dependent materials

| FEATURES IN THIS EXAMPLE                                       |  |
|--|--|
| • Creating composition or temperature dependent material files | • OC Library Mode                      |
| • Opt. Const. Compare Model<br>(OC Compare)                    | • <a href="#"><u>Build Library</u></a> |
| • <a href="#"><u>Draw Graph</u></a>                            |  |

In this example, we will demonstrate how to build a composition- or temperature-dependent optical constant library. This procedure can be used to create special material files for any series of samples that show a systematic shift in optical properties related to composition, temperature (or other material property or process condition). During the process, B-splines are used to smooth the constituent optical constant spectra for each known composition or temperature. The library is then built using an interpolation algorithm based on the critical point shifting algorithm of Snyder et al.<sup>4</sup> In the critical point shifting algorithm, the dielectric function at an arbitrary composition or temperature is evaluated from a weighted sum of the nearest reference dielectric function spectra, after the reference spectra are wavelength-shifted to line up the critical point features. CompleteEASE simplifies this process by automatically determining the wavelength shifting polynomials (that describe the path of critical points versus composition/temperature) via a non-linear regression analysis.

The full procedure for creating a composition or temperature dependent material file is to obtain optical constants from a series of samples with varying, known composition or temperature. This example will not demonstrate this initial step, as the procedures for each individual film will be similar to those taught in earlier examples. After successfully modeling the experimental data to determine accurate optical constants for a specific composition/temperature, save the tabulated optical constants for each material file. In this example, we work with a series of  $\text{Si}_{1-x}\text{Ge}_x$  material files that were obtained by fitting a series of layers with different germanium compositions (x). The actual composition was measured by other means – in this case XRD. Thus, we now have the optical constants (n,k) for a series of known  $\text{Si}_{1-x}\text{Ge}_x$  compositions.

Before starting this example, change the Wavelength Units to “eV”, and the Optical Constant Units to “e1 & e2” from the **Options** Tab.

<sup>4</sup> P.G. Snyder, J.A. Woollam, S.A. Alterovitz, and B. Johs, “Modeling  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  Optical Constants as Functions of Composition”, *J. Appl. Phys.* **68** 11 (1990) 5925.

## Opt. Const. Compare Model

To start this example, open the “Opt. Const. Compare” model from the Advanced Folder location. The model should appear as shown in Figure 5-73. Press the ADD MATERIAL line seven times to add seven layers to the model. Each of these layers will be used to hold the optical constants for a specific composition of  $\text{Si}_{1-x}\text{Ge}_x$ . Click on each layer where it says none to add a material file for that layer. There are 10  $\text{Si}_{1-x}\text{Ge}_x$  material files in the Examples Folder that were measured from a series of thin films with known composition (as determined from XRD). In addition, we can use crystalline Silicon and Germanium as the end-points for this material file. The compositions related to each material file are provided in Table 5-3.

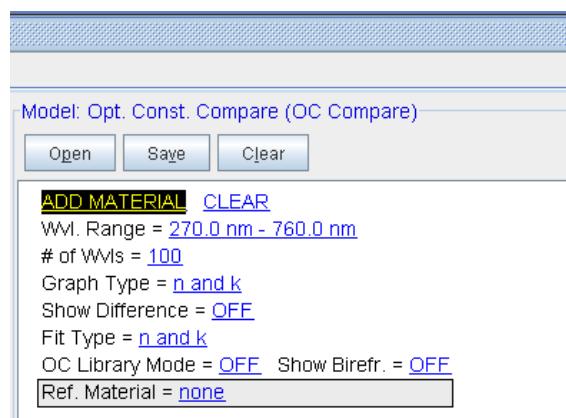


Figure 5-73. Opt. Const. Compare model.

Table 5-3. Compositions for each  $\text{Si}_{1-x}\text{Ge}_x$  material file used in this example.

| MATERIAL FILE NAME | GERMANIUM COMPOSITION % (X) |
|--------------------|-----------------------------|
| Si_jaw.mat         | 0% (x=0.000)                |
| SiGe-1.mat         | 5.2% (x=0.052)              |
| SiGe-2.mat         | 9.8% (x=0.088)              |
| SiGe-3.mat         | 15.5% (x=0.155)             |
| SiGe-4.mat         | 20.4% (x=0.204)             |
| SiGe-5.mat         | 26.3% (x=0.263)             |
| SiGe-6.mat         | 31.9% (x=0.319)             |
| SiGe-7.mat         | 37.1% (x=0.371)             |
| SiGe-8.mat         | 42.3% (x=0.423)             |
| SiGe-9.mat         | 49.3% (x=0.493)             |
| SiGe-10.mat        | 53.9% (x=0.539)             |
| Ge.mat             | 100% (x=1.000)              |

For this example, populate the seven layers with Silicon, SiGe-2, SiGe-4, SiGe-6, SiGe-8, SiGe-10, and Germanium (all shown in green in table). Before you will be able to set the compositions for each layer, you must turn ON the “OC Library Mode”. Type the corresponding compositions for each layer as shown in Figure 5-74. The temperatures can remain at 25° Celsius for all files. If we were making a temperature dependent file, we would adjust the corresponding temperatures to match each material file.

[ADD MATERIAL](#) [CLEAR](#)

Wvl. Range = [1.632 eV - 4.593 eV](#)

# of Wvls = [100](#)

Graph Type = [e1 and e2](#)

Show Difference = [OFF](#)

Fit Type = [e1 and e2](#)

OC Library Mode = [ON](#) Show Birefr. = [OFF](#)

|  |
|--|
| Material = <a href="#">Ge</a> x = <a href="#">1.000</a> t = <a href="#">25.00°C</a> <a href="#">DELETE</a> |
|--|

| Material = [sige-10](#) x = [0.539](#) t = [25.00°C](#) [DELETE](#) |
| Material = [sige-8](#) x = [0.423](#) t = [25.00°C](#) [DELETE](#) |
| Material = [sige-6](#) x = [0.319](#) t = [25.00°C](#) [DELETE](#) |
| Material = [sige-4](#) x = [0.204](#) t = [25.00°C](#) [DELETE](#) |
| Material = [sige-2](#) x = [0.088](#) t = [25.00°C](#) [DELETE](#) |
| Material = [Si\\_JAW](#) x = [0.000](#) t = [25.00°C](#) [DELETE](#) |
| Ref. Material = [none](#) |

[Build Library](#) Resolution (eV) = [0.050](#)

#### + Spectra Shifting Parameters

Figure 5-74. OC Compare model setup to build a Library for SiGe films of different composition.

Before proceeding to build the OC Library from these reference files, set the wavelength range to match the material file. For the SiGe material files, the optical constants were measured from 248nm to 1240nm (1eV to 5eV). Also, the “# of Wvls” may need to change to allow the B-Spline to more accurately match the reference files over this wide spectral range. The original material file contains about 540 individual wavelengths. Thus, I have set the “# of Wvls” to 500 – although this will significantly increase the amount of time needed for the calculation. When ready, press [Build Library](#), and a graph will appear as shown in Figure 5-75. In this graph, the colored curves are the reference optical constants at the specified compositions, and the black dashed curves are interpolated spectra at reference and midpoint compositions. Thus, each colored graph should be matched with a corresponding dashed black curve. The additional dashed black curves should demonstrate whether the “shifting” algorithm has worked.

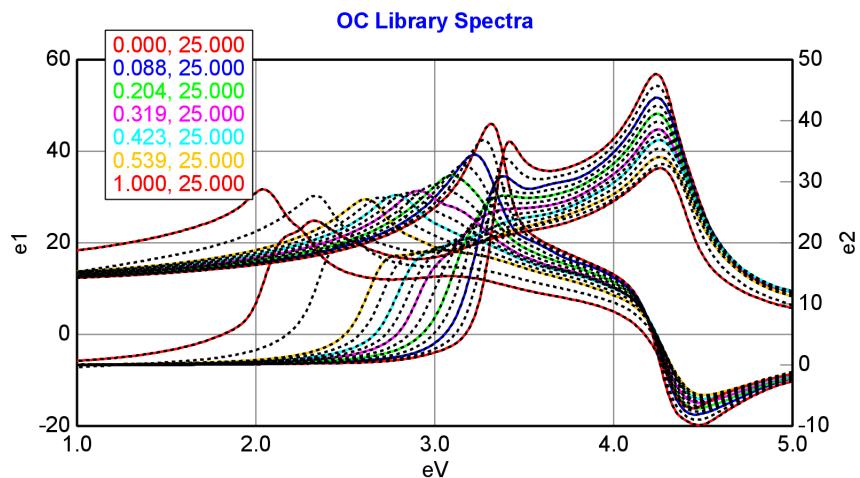


Figure 5-75. Results after building OC Library for SiGe.

## Draw Graph

This graph can be very busy, but you can change the view by selecting a different setting at the bottom of the model under **Draw Graph**. Pressing the [e1 & e2](#) selection will open the dialog box shown in Figure 5-76. Figure 5-77 and Figure 5-78 show the [e1 only](#) and [e2 only](#) spectra for this example, respectively. In addition, the graph can show the Shifted Spectra and Wvl Shift Function to help assess whether the composition library is successful. For advanced users, the Library Resolution and Spectra Shifting Parameters can be modified, as shown in Figure 5-79.

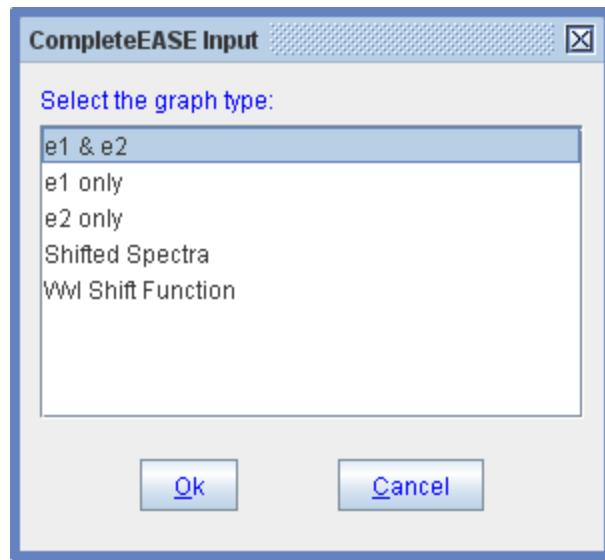


Figure 5-76. Graphing selections after building an OC Library.

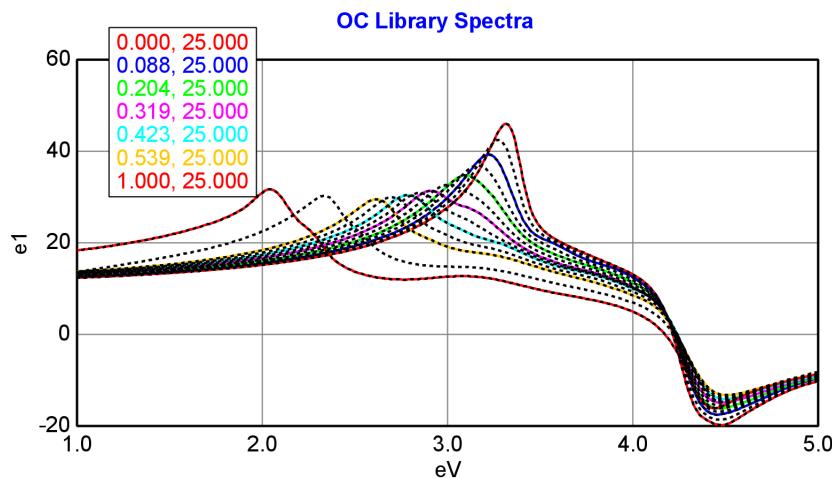


Figure 5-77. Graph of  $e1$  only after building the SiGe composition library.

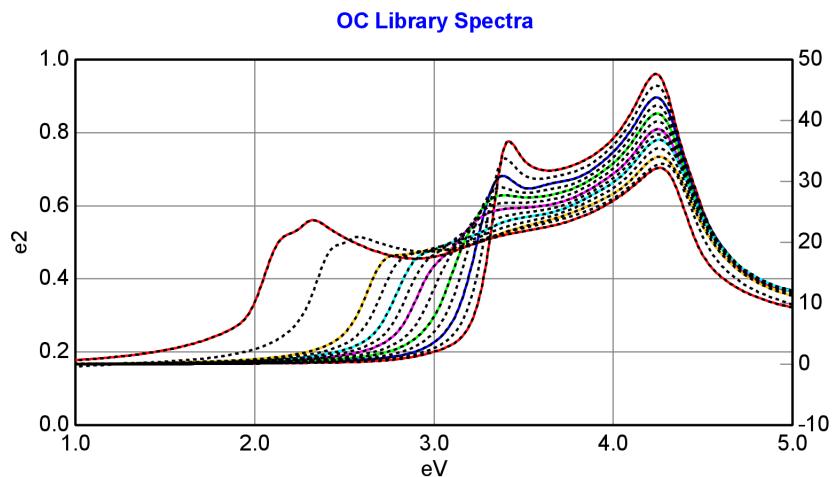


Figure 5-78. Graph of  $e2$  only after building the SiGe composition library.

**Build Library** Resolution (eV) = 0.050

**Spectra Shifting Parameters**

Wvl Order = 3

Max. Comp. Order = 3

Max. Temp. Order = 3

**Draw Graph** Graph Type: e2 only

**Save OC Library**

Figure 5-79. Advanced features to customize the OC Library algorithm, including spectral shifting parameters and resolution in eV.

To further assess whether the library algorithm was successful, you can zoom in on each of the graphs. Figure 5-80 shows a zoomed view of the E1 peak for the SiGe films. This shows that the peaks are shifted to higher energy with increasing silicon composition.

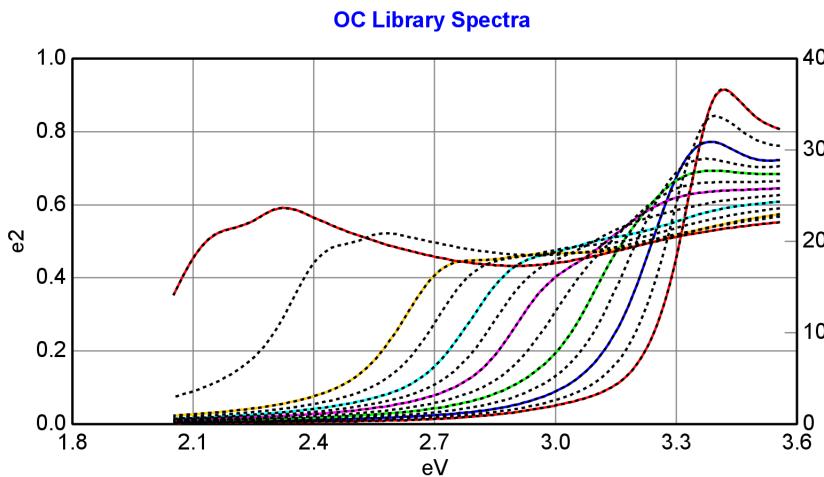


Figure 5-80. Zoomed view of the E1 peak for the SiGe compositions, showing a nice shift in critical point toward higher energy for increasing silicon composition.

## Save OC Library

After successful calculation of a composition or temperature dependent optical constant file, press **Save OC Library** at bottom of the Model panel. This material file can now be used to fit future data files. To demonstrate what this file looks like and how it operates, click the “Reference Material = none”, which is the bottom layer in our OC Compare model. Add your newly created material file in this entry. Change the Graph Type in the Model to e2 only and roll your mouse over the composition in this Reference Material. You will be able to visualize the optical constants shifting compared to your reference constants as the composition is varied. An example graph is shown in Figure 5-81, where the composition has been moved to x=0.75 to see how well the shifting works between the two most widely spaced reference values.

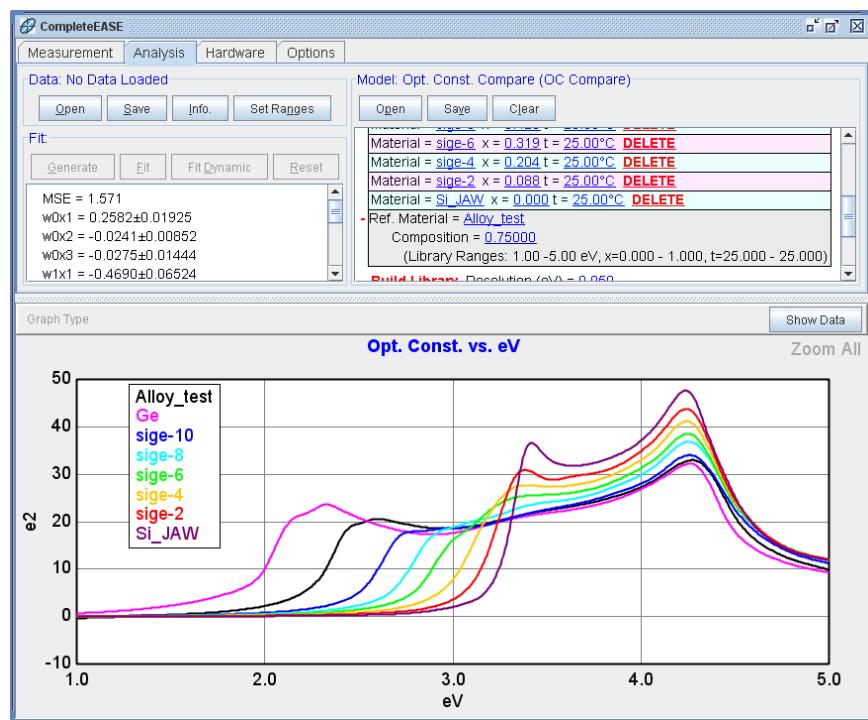


Figure 5-81. The newly created Composition dependent file has been added as the Reference material to compare to the original reference material as the composition is varied.

## 5.5. Anisotropic Films

| FEATURES IN THIS EXAMPLE                    |                   |
|---|-------------------|
| • Convert to Anisotropic<br>• Biaxial Layer | • Difference Mode |

In this example, we will allow a layer to have anisotropic optical constants, where the index normal to the sample surface is different than the index in the sample surface plane. This is common with many polymer films that orient along a specific direction due to processing.

To start, open the “Aniso-Organic on Si” data file from the Examples folder. The data should appear as shown in Figure 5-82. For simplicity, turn off the Double-Y Axis and view the Psi curves. The oscillations show that this film is transparent over the measured spectral range. Open the “Si with Transparent Film” model and press Fit. The results of this fit should appear as seen in Figure 5-83.

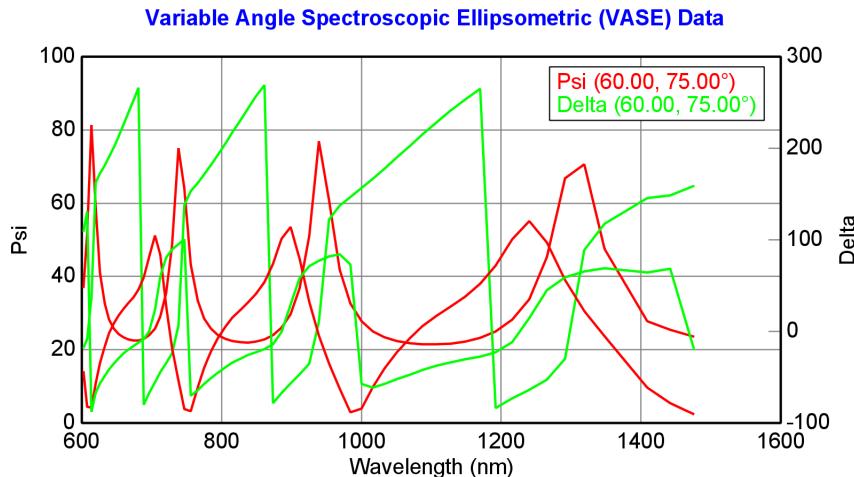


Figure 5-82. SE measurement from anisotropic organic film on silicon substrate.

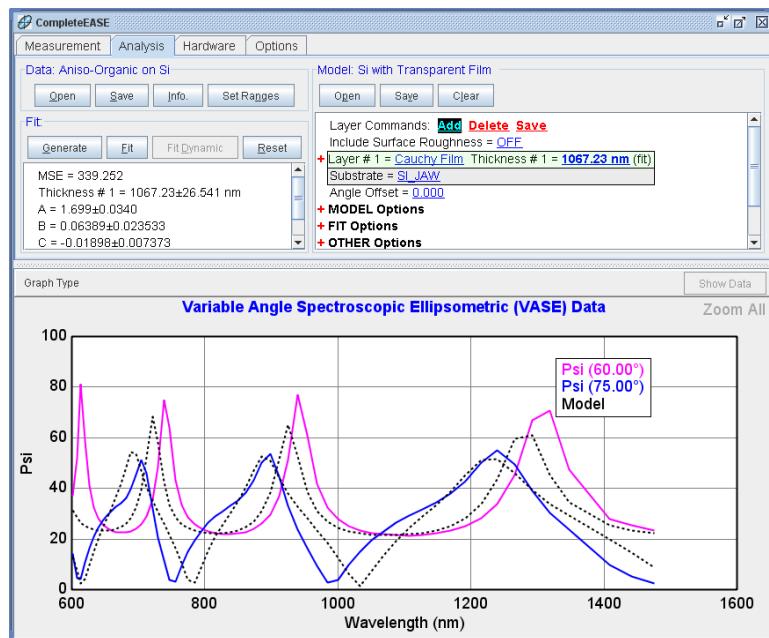


Figure 5-83. Fit to the anisotropic film using standard Transparent Film model.

Upon closer inspection, the data at 75 degrees shows a common “signature” of anisotropy in the film. The interference oscillations from anisotropic films will often “tilt” such that the curves are higher on one side of the peak and lower on the opposite side. This is demonstrated for anisotropic films on silicon at 75 degrees in Figure 5-84. The red curve represents an isotropic film. The green curves are higher on the long wavelength side of a peak and lower on the short wavelength side. These represent anisotropic films with  $N_z > N_{xy}$ . The blue curves are lower on the long wavelength side of a peak and higher on the short wavelength side. These represent anisotropic films with  $N_{xy} > N_z$ .

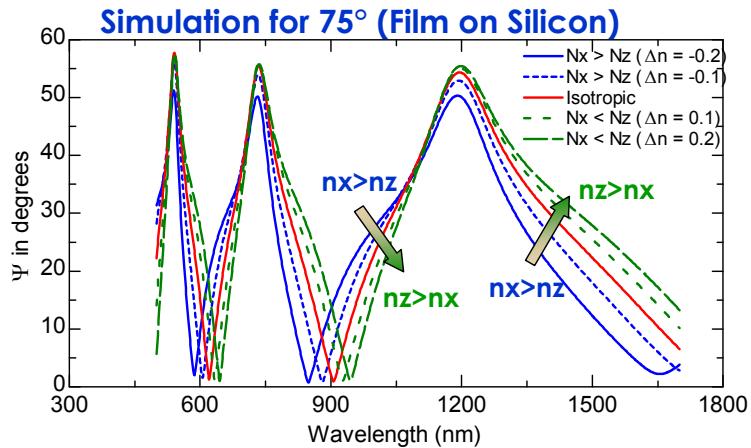


Figure 5-84. Simulation for transparent films showing the effects of anisotropy with either  $N_z > N_{xy}$  or  $N_{xy} > N_z$  as compared to isotropic data.

## Convert to Anisotropic

Right-click over Cauchy Film to access the menu of options to modify the Cauchy layer. From this list, choose to “Convert to Anisotropic”. The Cauchy layer will now become embedded as part of a new layer named “Biaxial”. Biaxial stands for anisotropy where Nx, Ny, and Nz are all different. However, the layer name is used here to describe any anisotropic film. Within the Biaxial layer, you can choose either Uniaxial or Biaxial anisotropy. For our case, we will use Uniaxial anisotropy, as it would require more advanced measurements to study the potential Biaxial anisotropy of a sample. This will be described in more detail in a later Example.

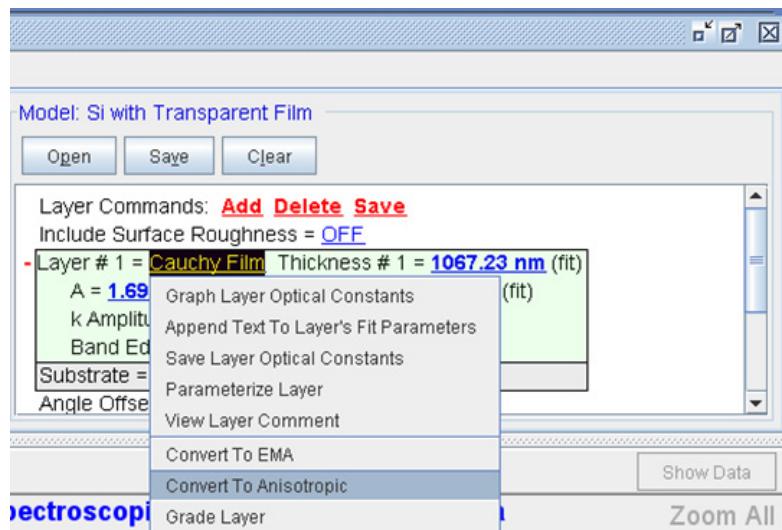


Figure 5-85. Right-click over the Cauchy Film to “Convert to Anisotropic”.

## Biaxial Layer

The biaxial layer can be used in two different ways and both will work equally well for this example. The difference is whether to have Difference Mode = OFF, as shown in Figure 5-86 or Difference Mode = ON, as shown in Figure 5-87.



Figure 5-86. Biaxial layer with Uniaxial anisotropy and Difference Mode OFF.

```

- Layer # 1 = Biaxial Thickness # 1 = 1067.23 nm (fit)
  Type = Uniaxial
  Optical Constants: Difference Mode = ON
    - Ex = Cauchy Film
      A = 1.699 (fit) B = 0.06389 (fit) C = -0.01898 (fit)
      k Amplitude = 0.00000 Exponent = 1.500
      Band Edge = 400.0 nm
    Index Differences:
      dZ_A = 0.000000 (fit) dZ_B = 0.000000 (fit) dZ_C = 0.000000 dZ_D = 0.000000 dZ_IR = 0.000000
    Euler Angles: Phi = 0.000 Theta = 0.000
  Substrate = SI_JAW

```

Figure 5-87. Biaxial layer with Uniaxial anisotropy and Difference Mode ON.

With the Difference Mode = OFF, each direction is described by an individual layer. In our case, each direction is seeded with the Cauchy layer, as that is the layer we started with. The layers could just as easily be B-Spline, Gen-osc, or a mixture of these.

With the Difference Mode = ON, the x-direction is defined by a material layer, while all other layers are determined by summing the x-direction optical constants with the “difference” value calculated from the extended Cauchy type dispersion described as the dZ (z-difference). This method can be extremely useful when the fit is primarily sensitive to the index difference and not sensitive to the absolute value of the index.

For this example, turn the Difference Mode to ON and then “roll” the mouse wheel over the dZ\_A parameter. If you roll this parameter to positive numbers, the simulated curve will look worse than the isotropic fit (tilt in wrong direction). However, if you roll the dZ\_A parameter to negative values, it will start to match better. Go ahead and fit the dZ\_A and dZ\_B parameters. Make sure you are still fitting the Cauchy parameters and the thickness, but it is wise to now turn off the Global Fit and Thickness Prefit, as we are close to the final answer. The final result should appear as shown in Figure.

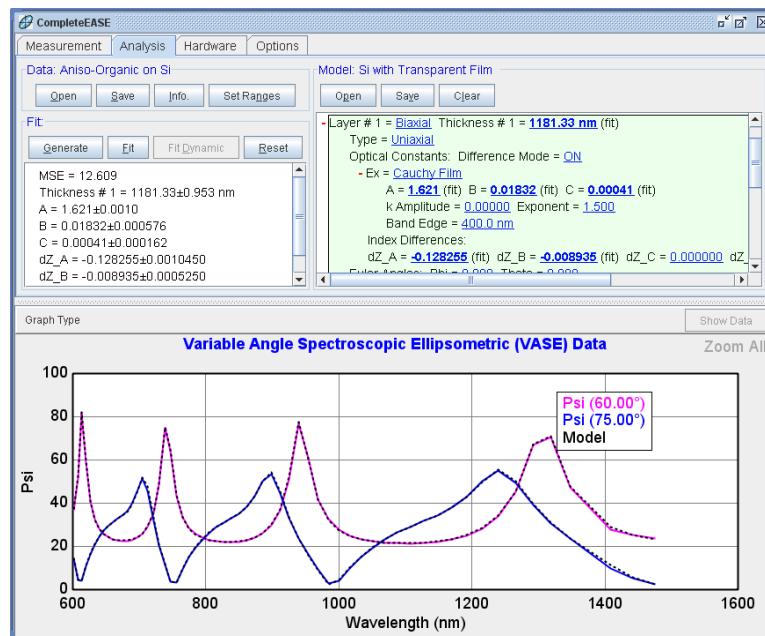


Figure 5-88. Anisotropic fit using the Difference Mode = ON.

---

## **5.6. Generalized SE and Mueller-Matrix Analysis**

Example is still under construction.

# 6. Reference - Graph

In this chapter, the features and capabilities of CompleteEASE will be described, using a “reference” format. That is, the features will be listed in the order they appear on screen, but not necessarily in the order one would use to perform typical procedures. The previous chapters on Basic System Operation and Data Analysis should be studied for “procedural” documentation.

## 6.1. Basic Screen Layout

The basic layout of the CompleteEASE software consists of Tabbed Panes across the top of the window, with a Graph always visible in the bottom section (Figure 6-1). The window can be resized, maximized, or minimized using standard Windows keystrokes or mouse operations. The divider bar between the Tab Panels and Graph can be moved to adjust the relative size of the graph. The CompleteEASE screen layout is saved when the program exits, and restored upon restart.

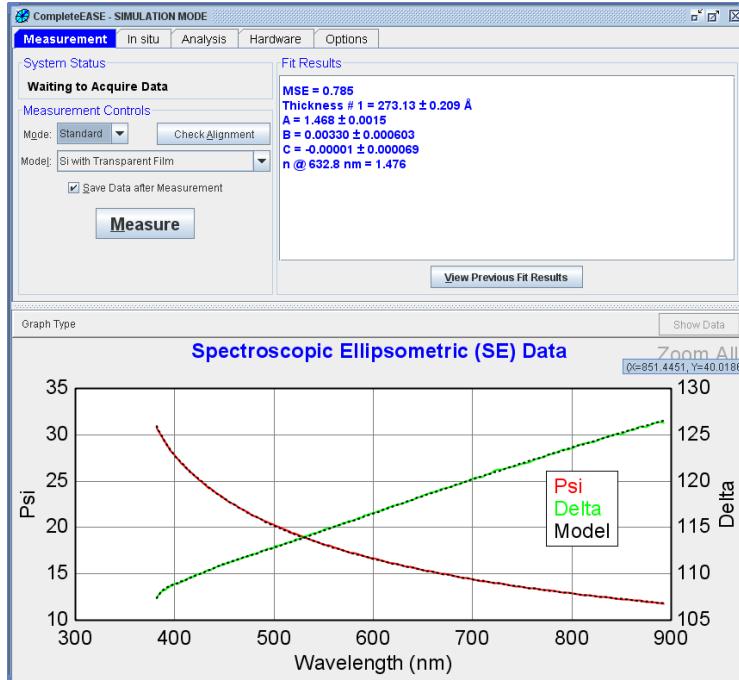


Figure 6-1. CompleteEASE software with the **Measurement** tab selected.

## 6.2. Graph Pane

The Graph pane is an important part of the CompleteEASE user interface. Spectroscopic data, model fits, and optical constants are all plotted in the Graph pane. The features described in this section can be used regardless of the type of information displayed in the graph window.

If the mouse is stopped in the plot area for a few seconds, a “tool tip” box will appear which reports the X and Y values corresponding to the mouse position. The mouse can be moved to other positions and the X-Y values will be updated.

The legend can be repositioned by clicking ( $\text{Ctrl} + \text{L}$ ) in the legend area and dragging the legend box to the desired location.

### ‘Show Data’

If optical constants (or something else besides data) are being graphed, you can press this button to go back to the data graph.

### Range-Select

To “zoom in” on a specific spectral range, hold down ( $\text{Ctrl} + \text{L}$ ) and drag over the desired spectral range (Figure 6-2). The graph will then redraw, plotting only the selected spectral range.

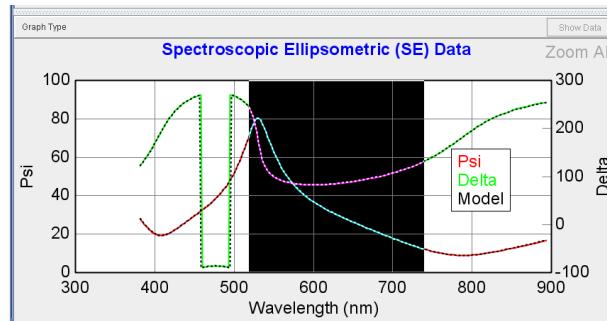


Figure 6-2. To select a specific spectral range (hold down the left mouse button and drag the mouse over the desired range).

### Zoom All

To plot the entire spectral range, simply press the ‘Zoom All’ button at top-right of the Graph pane (Figure 6-3). This same option can be found at the top of the Right-Click menu from within the graph.

NOTE: ‘Zoom All’ does not appear if you change the graph to “Use Clipboard Aspect Ratio”.

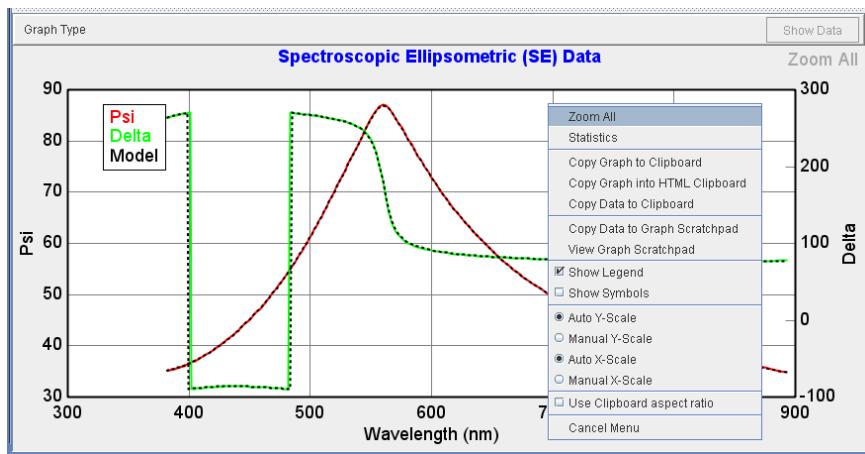


Figure 6-3. Right-Mouse menu from within the Graph.

## Right-Click Menu (Graph)

Press ( $\text{Ctrl}+\text{R}$ ) in the graph area to access the menu shown in Figure 6-4.

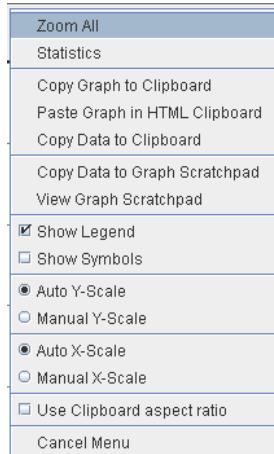


Figure 6-4. Right-click ( $\text{Ctrl}+\text{R}$ ) menu from Graph pane.

### Zoom All

Press to graph all data.

### Statistics

The graphed data undergo a variety of statistical calculations. For example, a straight-through measurement of air can be used to verify the measurement accuracy. The statistics of this measurement can then be calculated, as in Figure 6-5.

| Graph Statistics |          |           |          |          |          |         |             |
|------------------|----------|-----------|----------|----------|----------|---------|-------------|
| Parameter        | Average  | Std. Dev. | Slope    | Minimum  | Maximum  | Range   | # of Points |
| Psi              | 44.99876 | 0.01579   | -0.00008 | 44.96774 | 45.05014 | 0.08239 | 188         |
| Delta            | -0.00625 | 0.02119   | 0.00002  | -0.13881 | 0.07593  | 0.21475 | 188         |

Figure 6-5. Graph Statistics, taken from a straight-through measurement.

### **Copy Graph to Clipboard**

Graph is copied to the clipboard for use in other programs.

### **Paste Graph in HTML Clipboard**

The HTML Clipboard is used in CompleteEASE to compile a series of graphs or results. The HTML Clipboard can be viewed from the *Analysis>Fit:* pane.

### **Copy Data to Clipboard**

Graphed data curves are copied to the clipboard for use in a spreadsheet. Information will include a title line that matches the graph title; followed by columns of information with a heading for each column. The first column is the x-axis information – typically wavelength, followed by a column of information for each curve on the graph.

### **Copy Data to Graph ScratchPad**

Place the data curves from graph into a ScratchPad where they can be viewed and compared to other curves, along with customization of the curves being viewed.

### **View Graph ScratchPad**

The Graph ScratchPad is a convenient place internal to CompleteEASE to compare curves. The curves can be any type of data that is graphed, including raw data, model-generated curves, optical constants, or even the MSE profile from a Parameter Uniqueness test. An example of the Graph ScratchPad is shown in Figure 6-6.

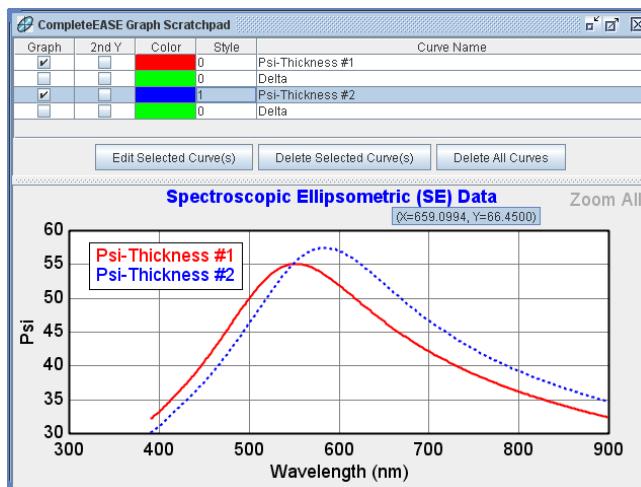


Figure 6-6. The Graph ScratchPad can be used to compare all types of graph curves, and customize the view for easier comparison.

## Show Legend

Turn On/Off the graph legend.

## Show Symbols

Turn On/Off graph symbols for the Experimental Data. The model curves are still represented as solid lines. Figure 6-7 shows an example data graph with symbols on.

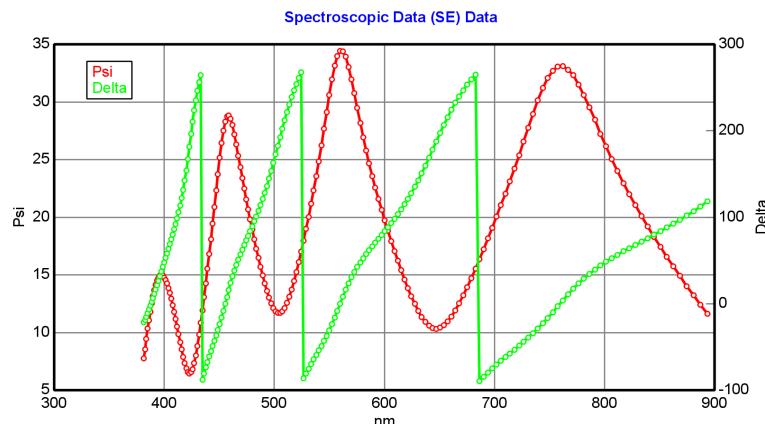


Figure 6-7. Graph with symbols turned on.

## Auto Y-Scale

Y-Axis is automatically selected to show all data.

## Manual Y-Scale

User can select lower and upper Y-axis limits. All data are still included when fitting, but only points within this range are graphed.

## Auto X-Scale

X-Axis is automatically selected to show all data.

## Manual X-Scale

User can select the lower and upper X-axis limits. All data are still included when fitting, but only points within this range are graphed.

## Use Clipboard Aspect Ratio

The standard graph will scale with the size of the graph pane. However, when the graph is copied to the clipboard, it always uses the configured aspect ratio. Choose this button to view the graph as it will appear when copied to the clipboard. The clipboard aspect-ratio can be modified under the “Graph ClipboardParms” section of [Options>Configuration Controls:> ‘Edit Configuration’](#).

## Cancel Menu

Close the Graph menu.

# 7. Reference - Measurement Tab

The **Measurement** tab is shown in Figure 7-1. This tab consists of three panels: **System Status**, **Measurement Controls**, and **Fit Results**. A brief description of all commands within this tab is provided.

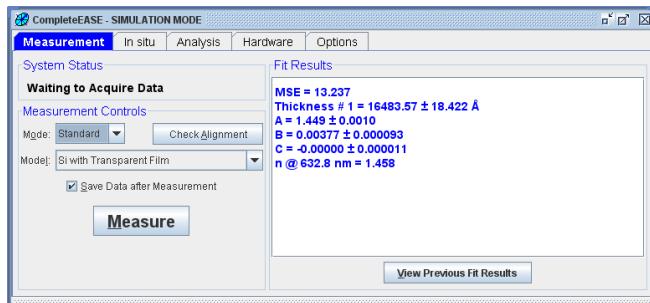


Figure 7-1. *Measurement Tab*

---

## 7.1. System Status Panel

This panel describes the current hardware status. Before the ellipsometer is ready to measure, the message will state “Not Initialized”. If the ellipsometer is ready for operation, “Waiting to Acquire Data” will be displayed.

---

## 7.2. Measurement Controls Panel

### Mode:

Specifies the type of measurement to collect:

Table 7-1. *Measurement Modes for alpha-SE systems.*

| MODE:    | DATA TYPE, TIME REQUIRED   |
|----------|----------------------------|
| Fast     | Ellipsometry, ~ 3 seconds  |
| Standard | Ellipsometry, ~ 10 seconds |
| Long     | Ellipsometry, ~ 30 seconds |

|              |                                      |
|--------------|--------------------------------------|
| Transmission | Transmission Intensity, ~ 10 seconds |
| M.M.         | Mueller-Matrix, ~ 10 seconds         |
| M.M. Long    | Mueller-Matrix, ~ 30 seconds         |

For the “Standard” and “Long” modes, the motor home sensors are checked before and after measurement. Also, they both implement Zone—averaging, which collects data with input polarizer set to +45° and -45° and then reports the average. This improves data accuracy.

The M.M. data modes allow measurement of 12 Mueller matrix elements. The absolute intensity of m11 is measured, while all other elements are normalized to m11.

To improve accuracy of Transmission Intensity and Mueller matrix measurements, perform an “S-T Baseline” or “Off-Sample Baseline” prior to the sample measurement (from the **Hardware** tab).

## Sample Alignment:

Specifies how the Z-stage should be used to adjust the sample height before the measurement. Table 7-2 provides details for each choice.

*Table 7-2. Alignment Options*

| OPTION        | DESCRIPTION   |
|---------------|---|
| None          | Stage remains at current location, which is below beam for straight-through (90°) measurements.   |
| Standard      | Use for standard reflected measurements. This setting does a quick search for the light beam near the previous alignment position.                  |
| Robust        | A thorough alignment of the light beam that searches over the full translation range. Use for glass substrates with multiple reflected beams.       |
| Fixed Height  | Moves sample stage to height described in hardware configuration file.  |
| Prompt Height | Allows user to enter the sample stage height for measurement. Perform a z-stage scan from <b>Hardware</b> tab to help determine appropriate height. |

## Model

Specifies which model will analyze the data. If it is set to “None”, data will be acquired, but no data analysis will be performed.

## Save Data after Measurement

Check this selection to insure the data are saved after each measurement. The default setting for this option is ON, but it is “sticky” and will retain its new value until the program is turned off.

## ‘Measure’

Begins a measurement using the settings specified in the “Mode:” and “Sample Alignment.” fields. After data is acquired, the “Model:” is used to analyze the data. Results are placed in the box in the upper right corner of the screen.

---

## 7.3. Fit Results Panel

Data analysis results are placed in this text box, located in the upper right corner of the screen.

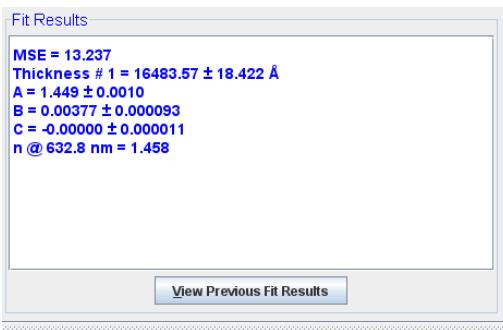


Figure 7-2. Fit Results panel in the Measurement Tab.

---

## 7.4. Right-click menu (**Measurement>Fit Results:**)

### Copy to Clipboard – Formatted

Copy results to the clipboard in a format ready to paste into a word processor, as shown below.

**MSE = 2.837**

**Thickness # 1 = 96.71 ± 0.018 nm**

**n of Cauchy Film @ 632.8 nm = 1.865**

### Copy to Clipboard - Table

Copy results to the clipboard in a format ready to paste into a table or spreadsheet, as shown below.

| PARAMETER                   | VALUE | ERROR BAR |
|-----------------------------|-------|-----------|
| MSE                         | 2.837 |           |
| Thickness # 1 (nm)          | 96.71 | 0.018     |
| n of Cauchy Film @ 632.8 nm | 1.865 |           |

## 7.5. ‘View Previous Fit Results’

Review results from past samples. This button will open a new dialog box, as shown in Figure 7-3. Choose the **Location** and **Files** you wish to review and a table of results is shown in the **File Information** panel. This table can be copied to the clipboard with the ‘Copy Text to Clipboard’ and ‘Copy Table to Clipboard’ buttons.

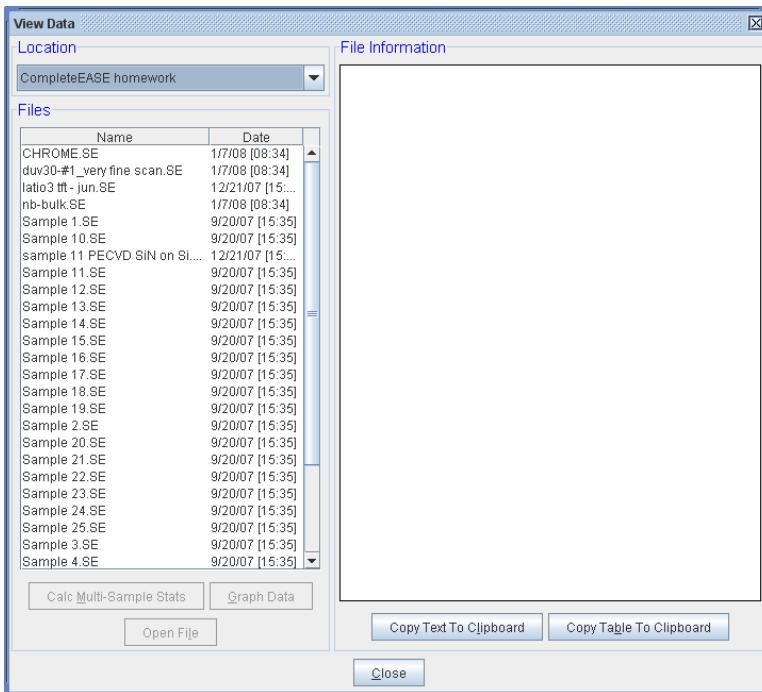


Figure 7-3. View Previous Fit Results Dialog box.

Select a single data file from the **Files** panel and you can ‘Open File’. This will open the data file, but not the model that was associated with the previous fit.

Use the mouse to select multiple results in the **Files** panel and you will be allowed to ‘Calc. Multi-Sample Stats’. An example of this is shown in Figure 7-4.

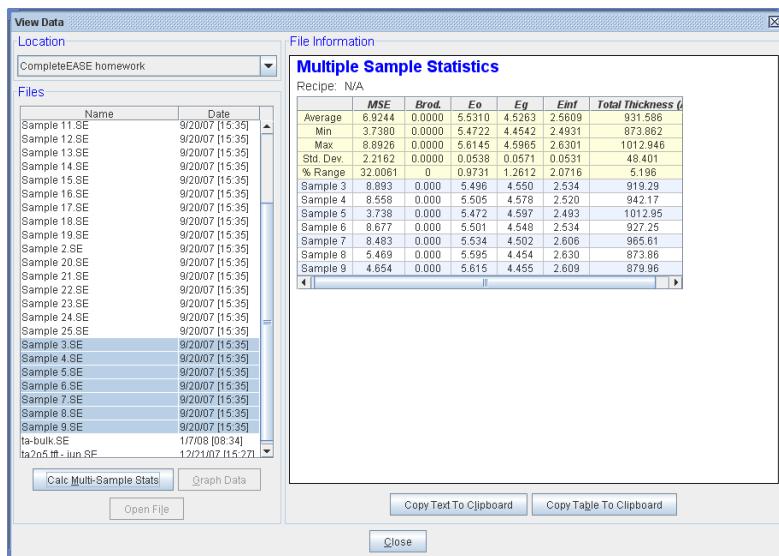


Figure 7-4. Viewing statistics from multiple samples.

If the selected data file is a map of multiple points across the sample, the ‘Graph Data’ button appears. When selected, a new window appears that allows the user to select the fit result they wish to view, as shown in Figure 7-5.

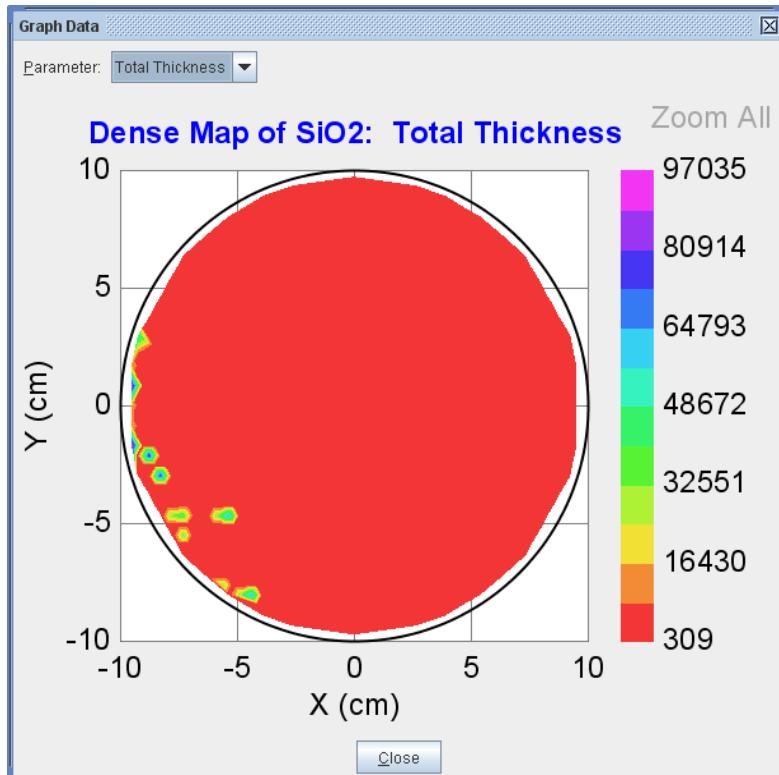


Figure 7-5. Uniformity map of total thickness.

# 8. Reference - Analysis Tab

The **Analysis** tab is shown in Figure 8-1. This tab consists of three panels: **Data**, **Model**, and **Fit**.

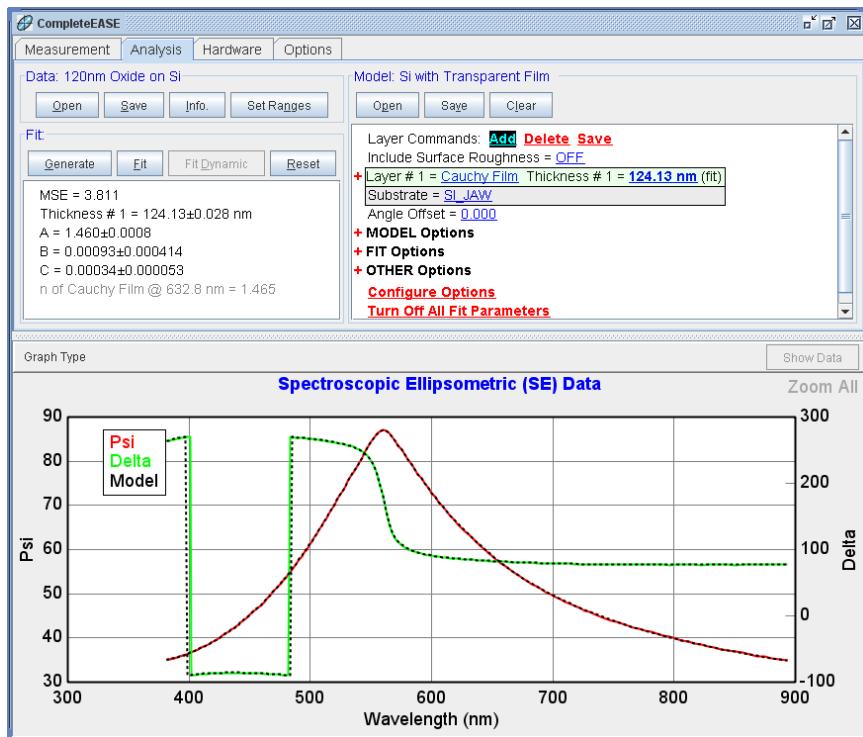


Figure 8-1. CompleteEASE software with the **Analysis** tab selected.

## 8.1. Data: Panel

### 'Open'

(**Ctrl**L): Open a data file.

(**Ctrl**R): “Append Data” file to existing data. The data files must share the same wavelengths.

## **‘Save’**

(**⌘L**): Save a data file.

(**⌘R**): Choose to “Save Data Subset” or “Export to Text File”.

### **“Save Data Subset”**

Right-click on ‘Save’ to choose this option. The data subset will consist of the reduced data that are currently selected (wavelengths, angles, time, etc.).

### **“Export to Text File”**

Right-click on ‘Save’ to choose this option. Data will be exported to a text file.

## **‘Info’**

Shows information about the current data set opened in CompleteEASE. An example of the information box is shown in Figure 8-2.

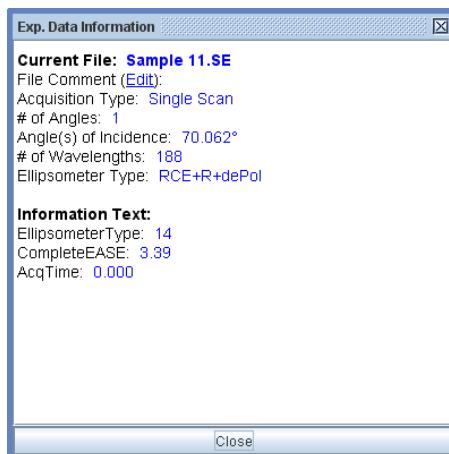


Figure 8-2. Information box showing details of data measurement.

## **‘Set Ranges’**

Choose the Minimum and Maximum wavelengths for use with current data set during fit.

---

## **8.2. Fit: Panel**

### **‘Generate’**

Generate data based on the current model and data set. Shortcut keystroke to Generate data is Alt-G.

### **‘Fit’**

Fit data based on the current model and data set. Shortcut keystroke to Fit data is Alt-F.

## **'Fit Dynamic'**

( $\text{^F}$ L): Fit dynamic data that has been taken versus time.

( $\text{^F}$ R): Choose to “Append Fit Results”, “Fit Backwards in Time”, or “Fit Backwards and Append”.

### **“Append Fit Results”**

When fitting Dynamic Data, it can be helpful to fit different regions of time separately. This menu option would be used after the first region has already been fit. The new range can be fit and appended to the previous fit results.

### **“Fit Backwards in Time”**

Use this option for dynamic data where the “end” result is better understood than at the beginning of the experiment. For example, it can be used for Etching studies, where the thickness at the last time is easier to determine.

### **“Fit Backwards and Append”**

This feature combines the previous two. It will perform the fit starting at the longest selected time and work backward – but then the results will be appended to previous dynamic data fit results.

## **'Reset'**

( $\text{^F}$ L): Restore the previous model parameters, from before the fit.

( $\text{^F}$ R): Choose to “Show Reset List”.

### **“Show Reset List”**

Provides a list of reset points that have been saved automatically by CompleteEASE before and after each “fit” since the most recent data/model have been in use. An example is shown in Figure 8-3.

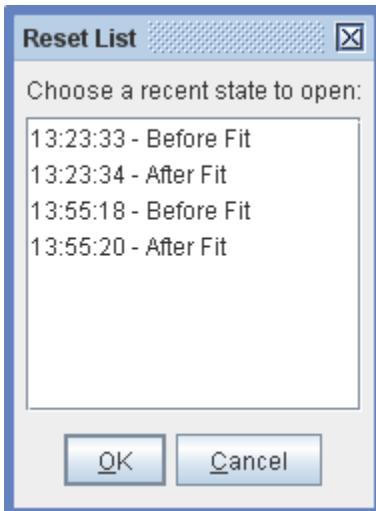


Figure 8-3. Reset List allows user to reset to any recent positions, which are automatically saved before and after each fit.

## 8.3. Model: Panel

The box in the right half of the tab displays all the options and specifications for the current data analysis model. An example model is shown in Figure 8-4. Details of each option within the model are given below.

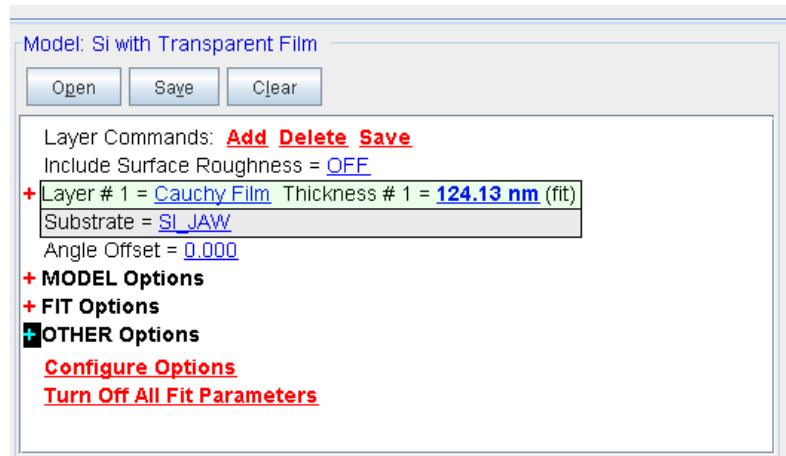


Figure 8-4. Basic **Model:** Panel in the *Analysis Tab*.

### ‘Open’

( $\text{⌘L}$ ): Open a new model.

( $\text{⌘R}$ ): Open Snapshot or Merge models.

#### “Open Snapshot”

Right-click on ‘Open’ button to open saved snapshots. A snapshot is a single file that compresses all information from the CompleteEASE screen, including the data measurement, model, and fit results. This is a convenient way to save and store information.

#### “Merge Models”

Right-click on the ‘Open’ button to merge models together.

### ‘Save’

( $\text{⌘L}$ ): Save current model and all model settings.

( $\text{⌘R}$ ): Save Snapshot.

#### “Save Snapshot”

Right-click on ‘Save’ button to save snapshot file. A snapshot is a single file that compresses all information from the CompleteEASE screen, including the data measurement, model, and fit results. This is a convenient way to save and store information. The file will be given “.ss” file extension.

## **‘Clear’**

Remove the current model.

## **Add**

Press this button to add a layer. The Add Layer to Model dialog box appears. Select the position of the new layer by moving the mouse to adjust the blue-bar and press the mouse button (Figure 8-5).

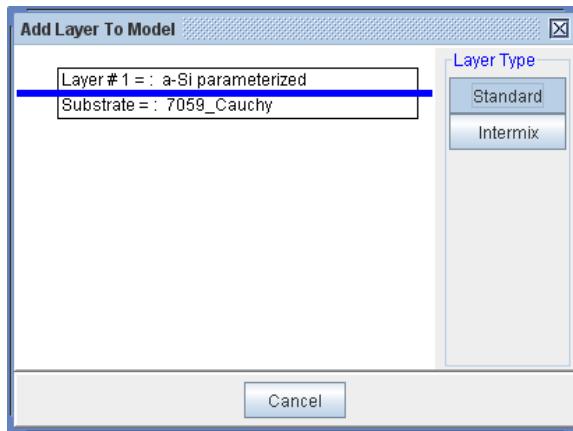


Figure 8-5. CompleteEASE “Add” dialog box.

## **Delete**

Press this button to delete a layer from the model. Choose the layer with the mouse (making it blue) and click to delete (Figure 8-6).

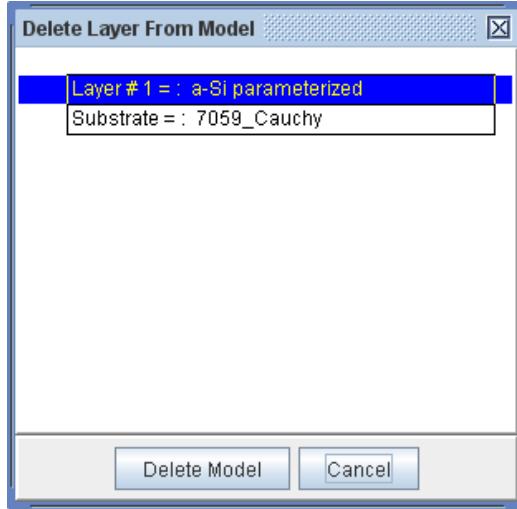


Figure 8-6. CompleteEASE “Delete” dialog box.

## Save

Press this button to save optical constants for a layer. Before clicking on the layer you wish to save (Figure 8-7), choose the Save Type (either Dispersion Parameters or Tabulated).

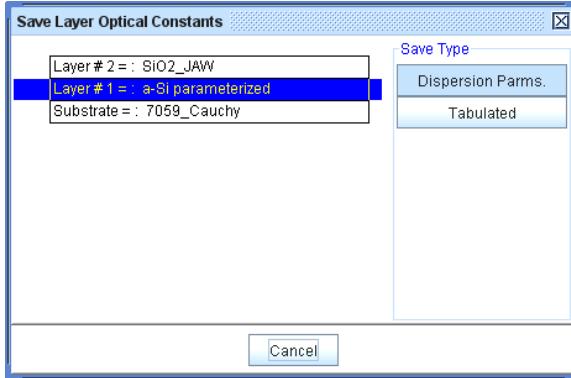


Figure 8-7. CompleteEASE “Save” dialog box.

## Include Surface Roughness

Turn on to fit a thin layer on the surface of existing model. The surface is modeled with a Bruggemann Effective Medium Approximation mixing the top film with 50% void. The only fit parameter available is the thickness of the rough surface. If the thickness moves to negative values, the roughness layer is modeled with -50% void mixing, which increases the surface region optical properties (rather than lowering them). The surface roughness layer is a “stealing” layer, in which it takes half of its thickness from the layer below. Thus, if a 100nm Cauchy layer has 20nm surface roughness on top, the model is actually calculated as 90nm Cauchy with 20nm surface roughness.

## Model Pictorial

The model is shown as a layer-by-layer picture with details regarding thickness and other parameters to describe the individual layers. Any layer with a “+” can be expanded to show more details about that layer. This is demonstrated in Figure 8-8.

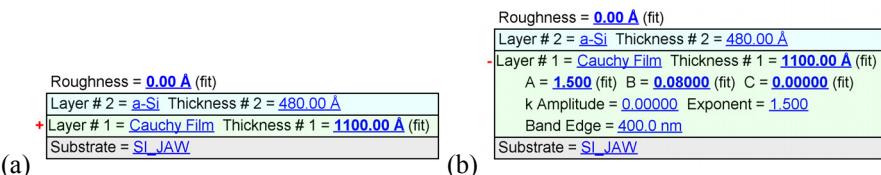


Figure 8-8. (a) Model with layers collapsed and (b) with Cauchy Film layer expanded.

## Editing Layers

Each layer has a name, show in blue. Place your mouse over the layer name to do the following:

( $\text{Ctrl}$ L): Open a new material file in place of the current layer.

(R): Choose from a menu to “Graph Layer Optical Constants”, “Append Text to Layer’s Fit Parameters”, “Save Layer Optical Constants”, “Parameterize Layer”, “View Layer Comment”, “Convert To EMA”, “Convert to Anisotropic”, or “Grade Layer”. This menu is shown in Figure 8-9

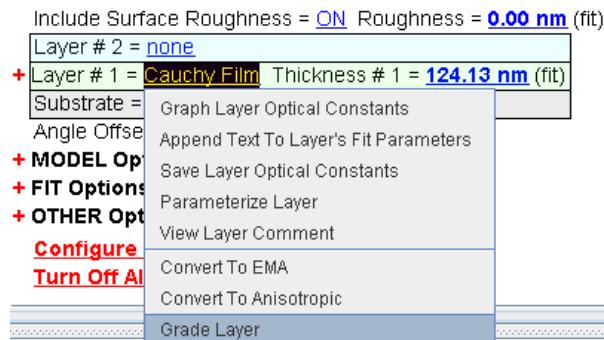


Figure 8-9. Right-click on a layer name to access this menu of options.

### **“Graph Layer Optical Constants”**

Right-click on a layer to select this option – the optical constants will be graphed.

### **“Append Text to Layer’s Fit Parameters”**

Right-click on a layer to select this option – the fit parameters will be reported with this additional text added.

### **“Save Layer Optical Constants”**

Right-click on a layer to save optical constants for that layer. You will be asked whether to save the Dispersion model parameters or a Tabulate list and then proceed to the File Location.

### **“Parameterize Layer”**

Right-click a layer to parameterize the optical constants of that layer using a dispersion model, such as the General Oscillator layer. This will open the layer optical constants as reference values in the Parameterize Layer dialog box, as shown in Figure 8-10.

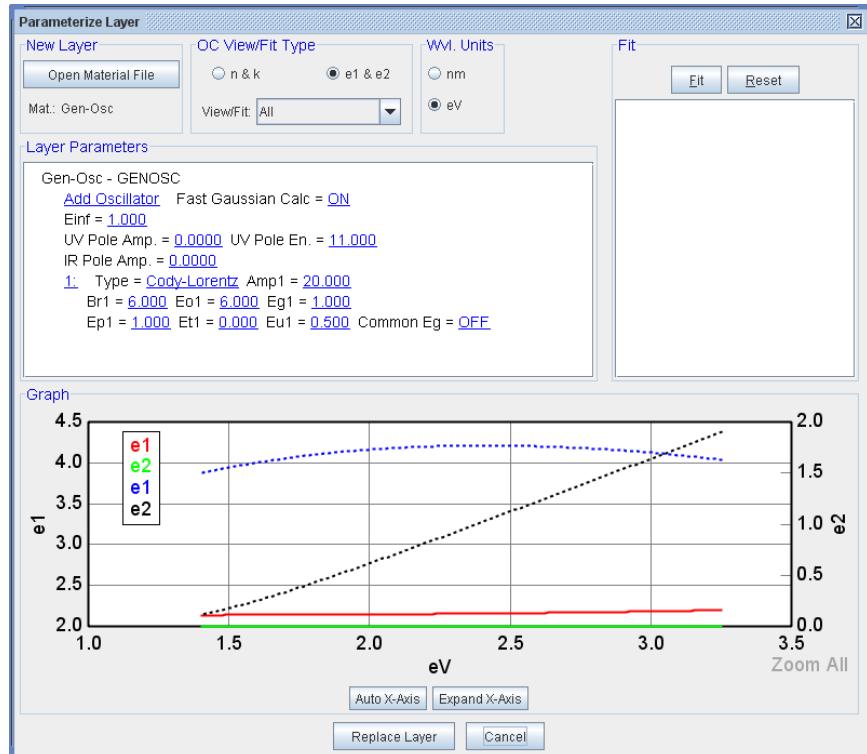


Figure 8-10. Parameterize Layer Dialog Box.

### **"View Layer Comment"**

Right-click and choose this option to view the layer comments, which often tell the source of the material file.

### **"Convert to EMA"**

Right-click to replace the layer with an EMA, in which the original layer is now embedded as the host material (Material 1). The second material is default to "Void" with EMA% default to 0, but selected as a fit parameter. An example is shown in Figure 8-11.

```
- Layer # 1 = EMA Thickness # 1 = 124.13 nm (fit)
# of Constituents = 2
+ Material 1 = Cauchy Film
Material 2 = VOID
EMA % (Mat 2)_james = 0.0 (fit)
depolarization_james = 0.333 Analysis Mode = Bruggeman
Substrate = SI_JAW
```

Figure 8-11. Example of the EMA layer where the Cauchy Film was automatically converted to the host (Material 1) with void as the second material.

### **“Unwrap from EMA”**

After converting a layer to EMA, you can right-click on the EMA layer to unwrap the host film back to a single layer without the EMA.

### **“Convert to Anisotropic”**

Right-click to replace the layer with an anisotropic Biaxial Layer, in which the original layer is now embedded as the starting material for both the Ex and Ez directions. The default configuration is to have no orientation (determined by Euler angles) and anisotropy set to Uniaxial ( $N_{xy} \neq N_z$ ). An example is shown in Figure 8-12.

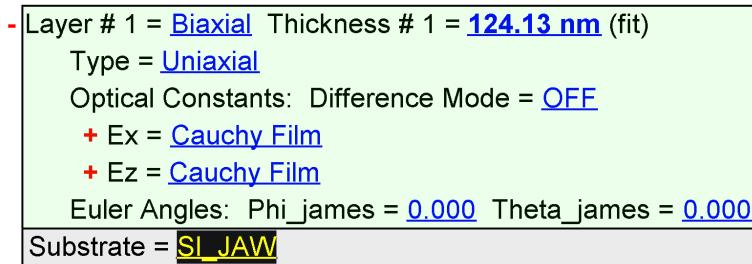


Figure 8-12. Example of Anisotropic layer.

### **“Convert to Isotropic”**

After converting a layer to Anisotropic, you can right-click on the Biaxial layer to unwrap the host film back to an isotropic layer.

### **“Grade Layer”**

Right-click to replace the layer with Graded Layer, where the original film is embedded as the average refractive index. The % inhomogeneity is default to 0%, but can be varied to allow the index to increase or decrease from the bottom to top of the layer. An example of this is shown in Figure.

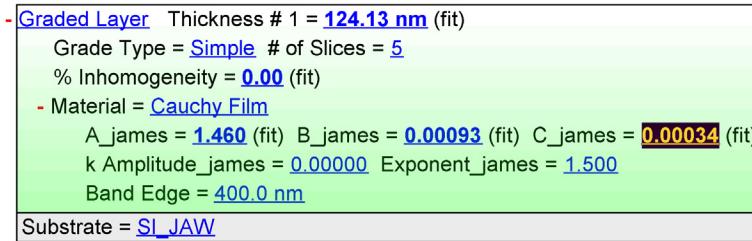


Figure 8-13. Example of Graded Layer.

### **“Remove Grading”**

After grading a layer, you can right-click on the Graded layer to unwrap the host film back to a layer without grading.

## **Angle Offset**

Apply an offset to the angle when calculating the model. This parameter can be fit.

---

## 8.4. Right-click menu (*Analysis>Model:*)

Right-click the mouse within the Model: Panel to access the menu options as shown in Figure 8-14.

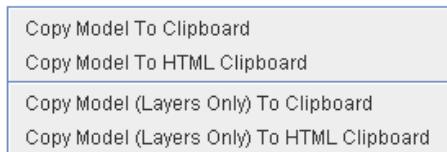


Figure 8-14. Right-click menu from within the *Model:* Panel.

### Copy Model To Clipboard

This option copies the entire Model to the Clipboard, including the Model Options, Fit Options and Other Options that are saved along with the Layer description. To view the details from a section, such as the Model Options, it needs to be expanded by pressing the “+” next to that section. An example of this “full” model is shown in Figure 8-15.

Layer Commands: [Add](#) [Delete](#) [Save](#)  
Include Surface Roughness = [ON](#) Roughness = [0.00 nm](#) (fit)  
+ Layer # 1 = [B-Spline](#) Thickness # 1 = [100.00 nm](#) (fit)  
Substrate = [SI\\_JAW](#)  
Angle Offset = [0.000](#)  
- MODEL Options  
    Include Substrate Backside Correction = [OFF](#)  
    Model Calculation = [Ideal](#)  
- FIT Options  
    + Perform Thickness Pre-Fit = [ON](#)  
    + Use Global Fit = [ON](#)  
    Fit Weight = [N.C.S](#)  
    Limit Wvl. for Fit = [OFF](#)  
    + Include Derived Parameters = [ON](#)  
- OTHER Options  
    [Wvl. Range Expansion Fit](#) Increment (eV) = [0.50](#)  
    [Try Alternate Models](#)  
    [Parameter Uniqueness](#)  
    Add Opt. Const. to HTML Report = [OFF](#)  
[Configure Options](#)  
[Turn Off All Fit Parameters](#)

Figure 8-15. “Full” Model as copied to Clipboard.

## **Copy Model To HTLM Clipboard**

This option copies the entire Model to the HTML Clipboard. The HTML Clipboard is used by CompleteEASE to compile results in a “report” format.

## **Copy Model (Layers Only) To Clipboard**

This option copies the Layered-description of a Model to the Clipboard. If you prefer to see a layer collapsed or expanded, make sure to pre-select your view before copying. An example of this model is shown in Figure 8-16.

Roughness = 0.00 nm (fit)

|  |
|--|
| + Layer # 1 = <u>B-Spline</u> Thickness # 1 = <u>100.00 nm</u> (fit) |
| Substrate = <u>SI_JAW</u>  |

Figure 8-16. “Layer-Only” Model as copied to the Clipboard.

## 8.5. Layer types

The CompleteEASE™ software provides many different ways to represent the optical constants of a material versus wavelength. These representations range from simple tabulated lists for the optical constants to complex dispersion models. All of these different representations are classified as layers in the CompleteEASE™ program. The layers currently available are listed in table 5.1. The rest of this chapter describes the operation and typical uses of the different layers in detail. This chapter makes extensive use of the OC Compare model to demonstrate the layers so reviewing that section of the *Working with Models* chapter would be advantageous.

Table 8-1. Layer types in CompleteEASE™.

| Layer Name               | Description  |
|--------------------------|--|
| Standard (Tabulated N,K) | Contains tabulated values for the optical constants of a material.   |
| Void                     | Contains optical constants for air (vacuum): n=1, k=0.   |
| EMA                      | A layer for mixing the optical constants of two materials together to create a composite material.   |
| EMA-Coupled              | A layer for mixing the optical constants of two materials together to create a composite material. In this case, the Material #1 is a “Coupled” layer which gets optical constants from a separate layer – referenced by the layer number.           |
| Cauchy                   | A simple dispersion layer using three terms to describe and index and an exponentially decaying function to describe the extinction coefficient.   |
| Cauchy_Wvl               | A simple dispersion layer using three terms to describe and index. In this special layer, the index can be defined at a specific “design” wavelength.  |
| Cauchy_Extended          | A simple dispersion layer using three terms to describe and index and an exponentially decaying function to describe the extinction coefficient.   |
| Sellmeier                | A simple dispersion layer useful for modeling dielectric materials.  |
| Coupled                  | Obtains optical constants from a separate layer in model.  |
| WvlByWvl                 | Allows optical constants to be individually determined on a wavelength-by-wavelength basis. This layer does not enforce Kramers-Kronig consistency and inherently contains a maximum number of fit parameters. Thus, it should be used with caution. |
| Biaxial                  | Layer to describe the anisotropic optical constants of both uniaxial and biaxial materials.  |
| Temperature/Alloy        | This layer contains optical constants of a material as a function of temperature and/or composition.   |
| General Oscillator       | A layer that allows multiple oscillators of various types to be used to represent the optical constants of a material.   |
| B-Spline Layer           | The B-Spline layer calculates a basis spline through evenly spaced points in eV for both $\epsilon_1$ and $\epsilon_2$ .   |

## Tabulated n,k

Most of the layers in the CompleteEASE™ material library are standard tabulated optical constant lists. The optical constants for this type are represented as a table of values versus wavelength. The table can contain the real and imaginary parts of the materials' dielectric function ( $\epsilon_1$  and  $\epsilon_2$ ) or the materials' complex index of refraction ( $n$  and  $k$ ). If the user finds optical constant tables in the literature and wishes to use them in CompleteEASE™, simply type the table into a file in the correct format and they can be opened.

Figure 8-17 shows how typical standard layers are represented in the Model. Unlike the rest of the layer types described in this chapter, these have no user adjustable parameters to define the optical properties making it the simplest layer type to use. Left clicking on the layer name ('SiO<sub>2</sub>\_JAW' in Figure 8-17) will bring up the 'Open Material' dialog allowing a different material to be chose for the layer. Right clicking on the layer name 'SiO<sub>2</sub>\_JAW' will open extended choices that include:

- "Graph Layer Optical Constants"
- "Append Text to Layer's Fit Parameters"
- "Save Layer Optical Constants"
- "Parameterize Layer"
- "View Layer Comment"
- "Convert to EMA"
- "Convert to Anisotropic"
- "Grade Layer"

These functions are the same for all layer types.

|   |  |
|---|--|
| Layer # 2 = <a href="#">SiO<sub>2</sub>_JAW</a> | Thickness # 2 = <a href="#">25.00 nm</a> |
| Layer # 1 = <a href="#">INTR_JAW</a>            | Thickness # 1 = <a href="#">1.00 nm</a>  |
| Substrate = <a href="#">Si_JAW</a>              |  |

Figure 8-17. A model constructed of standard layers – each set of optical constants is described by a table of values versus wavelength.

## Void

The Void layer is a special case of Tabulated N,K layer where the optical constants are fixed for all wavelengths at the nominal values for air (vacuum):  $n=1$ ,  $k=0$ .

## EMA

The EMA layer uses the Effective Medium Approximation to calculate the optical constants of a mixed material. Calculation is based on mixing optical constants of two or three constituent materials, the percentage of each material, a depolarization "screening" factor, and the calculation type. An EMA layer is shown in Figure 8-18.

The EMA layer in the EASE™ software provides three different EMA mixing methods for the user to choose. These include a simple Linear combination, Bruggemann EMA, and Maxwell-Garnet EMA. The Linear mixing simply interpolates between the constituents dielectric functions to get the optical constants

of the composite material. The Maxwell-Garnett and Bruggemann EMAs are more common. The Maxwell-Garnett assumes that spherical inclusions of materials #2 and #3 exist in a host matrix of material #1. The Bruggemann EMA makes the self-consistent choice of the host material. The Maxwell-Garnett and Bruggemann EMAs are very useful for modeling surface and interfacial roughness as well as modeling poly-crystalline materials by mixing together amorphous and crystalline optical constants of the material.

|   |
|---|
| - Layer # 1 = <a href="#">EMA</a> Thickness # 1 = <b>50.00 nm</b>       |
| # of Constituents = <b>2</b>  |
| Material 1 = <a href="#">a-si</a>                                       |
| Material 2 = <a href="#">Void</a>                                       |
| EMA % (Mat 2) = <b>23.0</b>   |
| depolarization = <b>0.333</b> Analysis Mode = <a href="#">Bruggeman</a> |

Figure 8-18. EMA model for mixed-constituent layers.

## EMA-Coupled

This is a special case of EMA layer, just as described above, except with the first material using the Coupled description. This allows the Material #1 to obtain optical constants from a separate layer in the model, designated by the layer number. An example of the EMA-Coupled layer is shown in Figure.

|  |
|--|
| - Layer # 3 = <a href="#">EMA-coupled</a> Thickness # 3 = <b>0.00 nm</b>       |
| # of Constituents = <b>2</b>   |
| - Material 1 = <a href="#">Coupled</a>   |
| Coupled to Layer # = <a href="#">2</a> (B-Spline)                              |
| Material 2 = <a href="#">Void</a>  |
| EMA % (Mat 2) = <b>50.0</b>  |
| depolarization = <b>0.333</b> Analysis Mode = <a href="#">Bruggeman</a>        |
| + Layer # 2 = <a href="#">B-Spline</a> Thickness # 2 = <a href="#">0.00 nm</a> |
| + Layer # 1 = <a href="#">Cauchy</a> Thickness # 1 = <a href="#">0.00 nm</a>   |
| Substrate = <a href="#">Si_JAW</a>   |

Figure 8-19. Example of the EMA-Coupled layer, where Material #1 receives its optical constants from a separate layer in the model, referenced by the layer number.

## Cauchy

The Cauchy layer is a commonly used layer for determining the optical constants of a transparent or partially transparent film (Dielectrics and Semiconductors below the fundamental bandgap). Over part of the spectral range, the optical constants of these materials can be represented by an index that varies slowly as a function of wavelength and an exponential absorption tail. The index of refraction of the Cauchy layer is represented by an inverse power series containing only even terms and the extinction coefficient is represented by a simple exponential tail. These representations are as follows:

The Cauchy is a dispersion layer that describes the index of refraction using a three-term equation, as in Equation 8-1. In addition to the three terms for index of refraction ( $n$ ), there are three additional terms to describe an Urbach absorption tail, as in Equation 8-2. The Cauchy layer and graph of the optical constants is shown in Figure 8-20.

$$n(\lambda) = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4} \quad (8-1)$$

$$k = k_{amp} \cdot e^{\exp(E-Bandedge)} \quad (8-2)$$

Figure 8-20 shows the Cauchy layer as displayed in the CompleteEASE model. The A, B, C parameters are variable fit parameters that determine the index dispersion. The *k Amplitude* and *Exponent* are fit parameters for determining the shape of the extinction coefficient dispersion. The *Band Edge* parameter can be set manually but is not a fit parameter since it is directly correlated to the *k Amplitude* parameter (the extinction coefficient is equal to *k Amplitude* at the *Band Edge*).

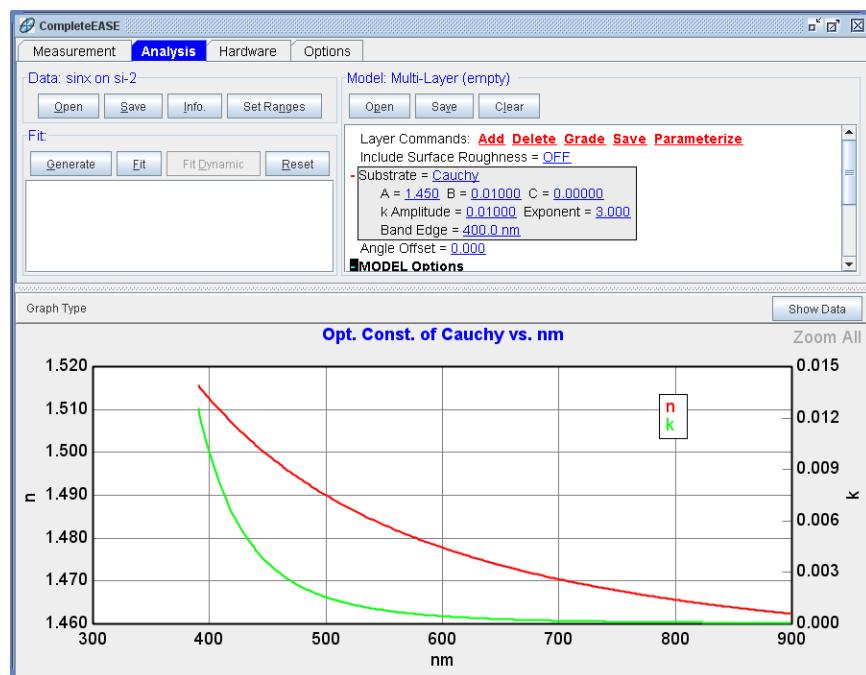


Figure 8-20. Cauchy dispersion layer in CompleteEASE.

## Cauchy\_WVL

This special representation of the Cauchy layer is found in the ADVANCED materials directory. It provides the same shape as the Cauchy, but is described with the terms shown in Figure 8-21. This allows the user to specify a known index of refraction at a specific wavelength, without concern for the dispersion terms.

- Substrate = Cauchy\_Wvl  
 n = 1.450 B = 0.01000 C = 0.00000  
 Design wvl = 632.8 nm

Figure 8-21. Cauchy\_Wvl layer is same dispersion shape as Cauchy, but allows entry of the index at a design wavelength in-place of the A parameter of the standard Cauchy.

## Cauchy\_Extended

This special representation of the Cauchy layer is found in the ADVANCED materials directory. It provides a similar shape to the Cauchy, but with ability to decrease index quickly toward NIR spectral region by adding an IR term. An example layer is shown in Figure 8-22 with the resultant optical constants shown in Figure 8-23.

- Layer # 3 = Cauchy\_Extended Thickness # 3 = 0.00 nm  
 A = 1.450 B = 0.00500 C = 0.00000  
 D = 0.00000 IR = 0.12000  
 Urbach Amplitude = 0.30000 Exponent = 2.000  
 Cody Amplitude = 0.200  
 Band Edge (eV) = 2.400

Figure 8-22. Example of the Cauchy\_Extended layer.

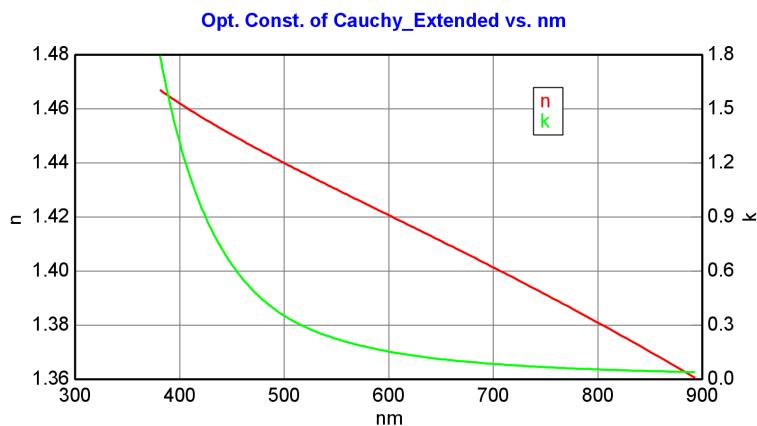


Figure 8-23. Optical constants from a Cauchy\_Extended layer.

## The Sellmeier Layer

The Sellmeier layer is another dispersion layer that can be used to represent dielectrics. It is used to represent the optical constants of transparent dielectric materials. CompleteEASE™ uses a 2-term Sellmeier model to account for UV and IR absorption. The representation for the index of refraction is:

$$n = \left( \varepsilon(\infty) + \frac{A\lambda^2}{\lambda^2 - B^2} - E\lambda^2 \right)^{\frac{1}{2}} \quad (8-3)$$

where  $\varepsilon(\infty)$  is an index offset,  $A$  is the amplitude,  $B$  is the center energy, and  $E$  is the position of a pole in the infrared. These are represented in the layer as ‘Einf’, ‘Amp.’, ‘Center En.’, and ‘IR Pole Amp.’ respectively. Figure 8-24 shows the layer as it appears in a model.

|  |
|--|
| - Substrate = <a href="#">Sellmeier</a>  |
| Amp. = <a href="#">0.743</a> Center En. = <a href="#">0.11000</a> IR Pole Amp. = <a href="#">0.01000</a> |
| Einf = <a href="#">1.000</a>   |

Figure 8-24. The Sellmeier layer as displayed in CompleteEASE model.

## Coupled

Special layer used to match the optical constants of a separate layer within the model. The Coupled layer expands to allow designation of the layer number where the optical constants should come from.

## WvlByWvl

Layer which allows the optical constants to vary independently at each wavelength. This layer has the utmost flexibility, but also the largest number of fit parameters. As it does not maintain Kramers-Kronig consistency or even smooth continuous curves for the optical constant dispersion, it should be used with extreme caution.

|  |
|--|
| - Layer # 3 = <a href="#">WvlByWvl</a> Thickness # 3 = <a href="#">100.00 nm</a>                               |
| Init. values: n = <a href="#">1.500</a> k = <a href="#">0.000</a> Starting Mat = <a href="#">none</a> 188 Pts. |
| Fit Opt. Const. = <a href="#">ON</a>   |
| Force E2 Positive = <a href="#">OFF</a>  |
| ShowParms = <a href="#">OFF</a>  |

## Biaxial

The biaxial layer allows the user to model anisotropic materials. This layer is used for both uniaxial and biaxial anisotropy and has 3 Euler-angle terms to rotate the orientation of optical axes relative to the ellipsometer measurement orientation. There are two modes which can be used within the Biaxial layer. With Difference Mode = OFF, the optical constants in all directions (2 for uniaxial, 3 for biaxial) are independently described by material files. This is shown in Figure. With Difference Mode = ON, the x-directed optical constants are described by a material file while an extended Cauchy “difference” is established for the index difference between the x-direction and the other orientations. This is shown in Figure.

- Layer # 2 = **Biaxial** Thickness # 2 = [0.00 nm](#)  
 Type = [Biaxial](#)  
 Optical Constants: Difference Mode = [OFF](#)  
 + Ex = [B-Spline](#)  
 + Ey = [B-Spline](#)  
 + Ez = [B-Spline](#)  
 Euler Angles: Phi = [0.000](#) Theta = [0.000](#) Psi = [0.000](#)

Figure 8-25. Biaxial anisotropic layer with Difference Mode = OFF

- Layer # 2 = **Biaxial** Thickness # 2 = [0.00 nm](#)  
 Type = [Biaxial](#)  
 Optical Constants: Difference Mode = [ON](#)  
 + Ex = [B-Spline](#)  
 Index Differences:  
 $dY_A = 0.000000$   $dY_B = 0.000000$   $dY_C = 0.000000$   $dY_D = 0.000000$   $dY_{IR} = 0.000000$   
 $dZ_A = 0.000000$   $dZ_B = 0.000000$   $dZ_C = 0.000000$   $dZ_D = 0.000000$   $dZ_{IR} = 0.000000$   
 Euler Angles: Phi = [0.000](#) Theta = [0.000](#) Psi = [0.000](#)

Figure 8-26. Biaxial anisotropic layer with Difference Mode = ON

## Graded Layer

All other layer types can be graded to model the optical variation with depth through the film. This is achieved via the GRADE button within the Model: panel. An example Graded Layer is shown in Figure 8-27. There are three types of grading that can be achieved in this layer: Simple, Linear, and Non-Linear. Grading is accomplished by dividing the thin film into a series of ‘slices’ that will have varying optical constants to approximate the index gradient profile. The number of slices can be designated. The primary fit parameter is the “% Inhomogeneity” which will be positive numbers when the index is larger toward the surface than the substrate and negative numbers if the index is smaller toward the surface. If you right-click on the title “Graded Layer”, the optical constants will be graphed, showing n and k at both top and bottom, as shown in Figure 8-28.

- Graded Layer Thickness # 1 = [0.00 Å](#)  
 Grade Type = [Simple](#) # of Slices = [5](#)  
 % Inhomogeneity = [0.00](#) (fit)  
 + Material = [cauchy](#)

Figure 8-27. Example of a Graded Layer.

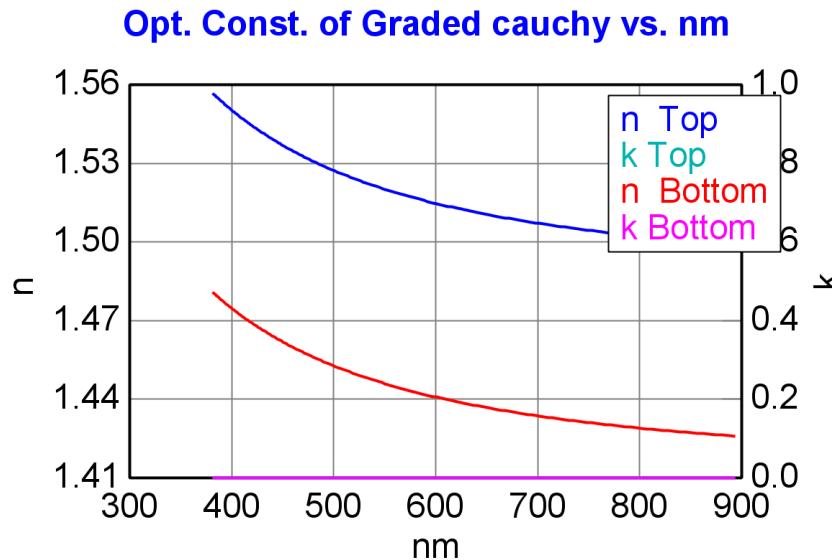


Figure 8-28. Graph of graded optical constants.

## Gen-Osc

The Gen-Osc layer is a General Oscillator material that allows the summation of different oscillator line shapes. Figure 8-29 shows a Gen-Osc layer with two oscillators of different types, along with associated graph of the resulting optical constants.

Within the Gen-Osc layer you can add a new oscillator by pressing “Add Oscillator”. To change the oscillator type, click on the “Type =” selection and you will get a dialog box with your choices, as in Figure 8-30. The various options are described in detail in an Appendix.

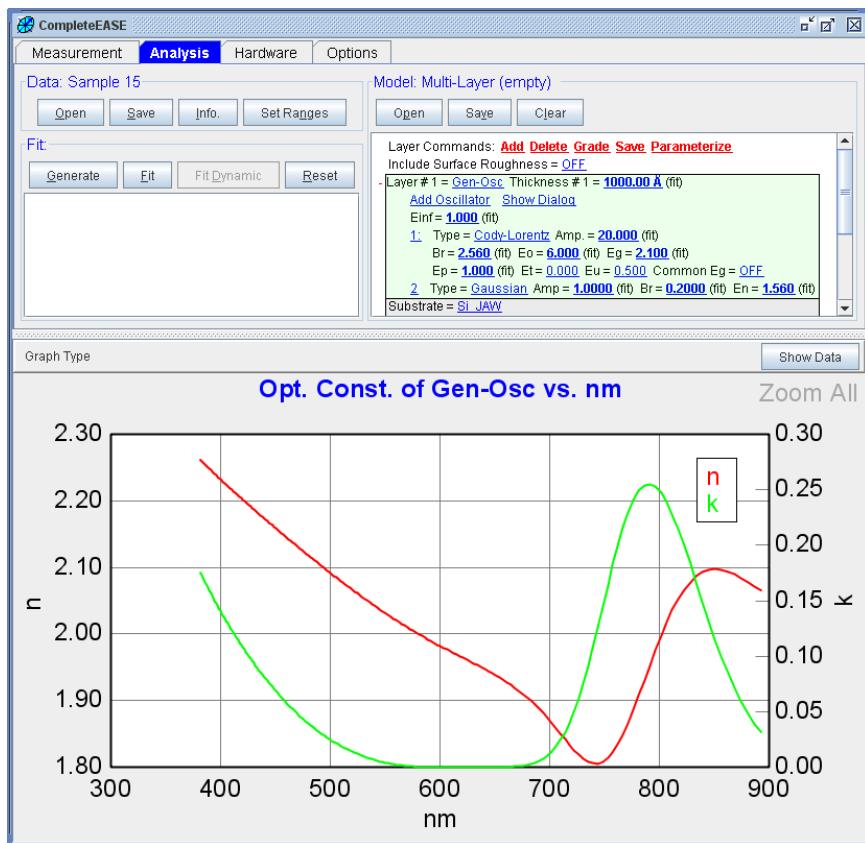


Figure 8-29. Gen-Osc dispersion layer with both a Cody-Lorentz and a Gaussian oscillator.

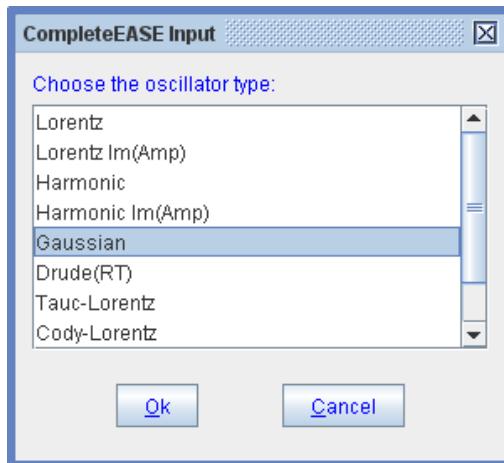


Figure 8-30. Choices for Oscillator Types within the Gen-Osc layer.

The General Oscillator layer currently supports many different types of oscillators: Lorentz, Harmonic, Gaussian, Tauc-Lorentz, and Cody-Lorentz, and Tanguy, and Drude type dispersion.

Press “Show Dialog” to bring up the Editor to visualize and manipulate the oscillator parameters. This dialog editor is shown in Figure 8-31.

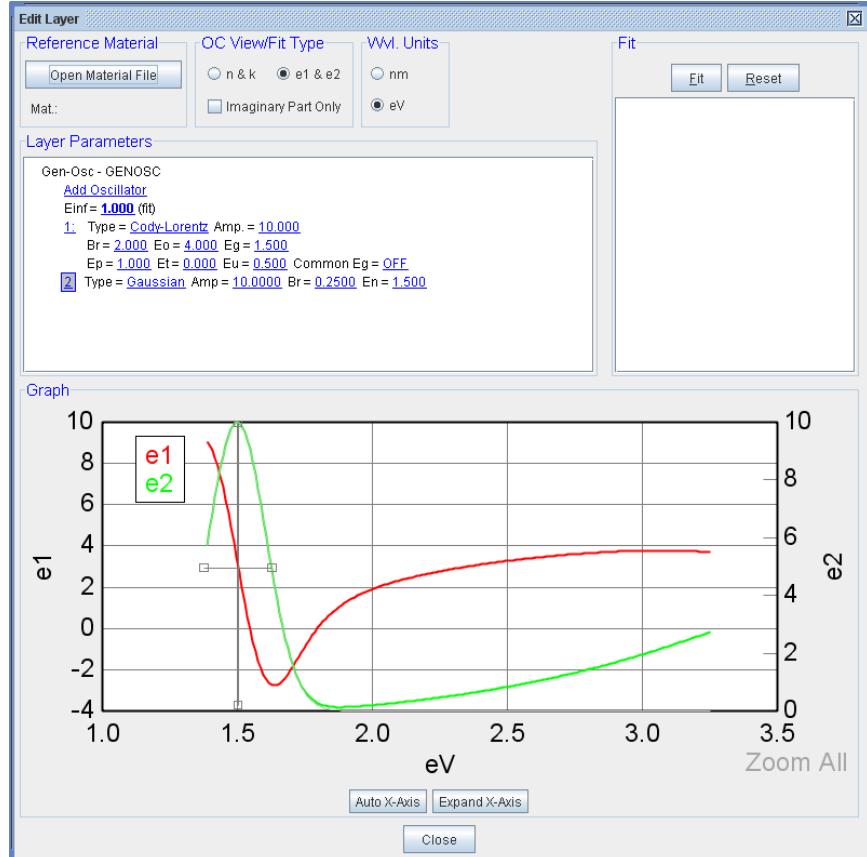


Figure 8-31. Dialog Editor to view and manipulate the Gen-Osc parameters.

The oscillators can be manipulated by pressing the number to their left. Use care when pressing the number, as each mouse-button does a different function:

(**Ctrl**R) Delete the oscillator from list.

(**Ctrl**L) Selects the oscillator and shows gray “drag-boxes” to allow manipulation of the oscillator parameters on graph.

The Dialog Editor allows the oscillator parameters to be matched to reference optical constants. This procedure is demonstrated in the Analysis Example on use of the Gen-Osc layer.

Further details regarding the Gen-Osc Layer are given in the next section.

## B-SPLINE

The B-Spline layer specifies the optical constants versus wavelength using a series of control points which are equally spaced in photon energy (eV). The approximate spacing of the control points is controlled by the “Resolution (eV)” field and the resulting number of control points within the current spectral range is listed after this value. Basis spline curves (which are by definition smooth and continuous in the 0th, 1st, and 2nd derivatives) are used to interpolate between the control points.

Clicking on the “Draw Node Graph” displays the location of the spline control points. The B-Spline layer always works in terms of the complex dielectric function  $\epsilon = \epsilon_1 + i\epsilon_2 = (n + ik)^2$ , which is often written as “e1 & e2”. One set of control points (and associated spline curve) is used to specify the dispersion in “e1” and a second set of control points is used to describe “e2”. Using a smaller “Resolution” value adds more control points, resulting in more flexibility to accommodate sharper features in the dielectric constant spectra. However, setting the Resolution too low can result in unwanted noise or unphysical artifacts in the dielectric function spectra.

The B-Spline will start with all nodes set to the Initial Values, as described within the layer. However, a “Starting Mat” can be entered and the spline points will automatically match the optical constants from this reference file. Figure 8-32 shows the B-Spline layer and spline points matched to Germanium starting material.

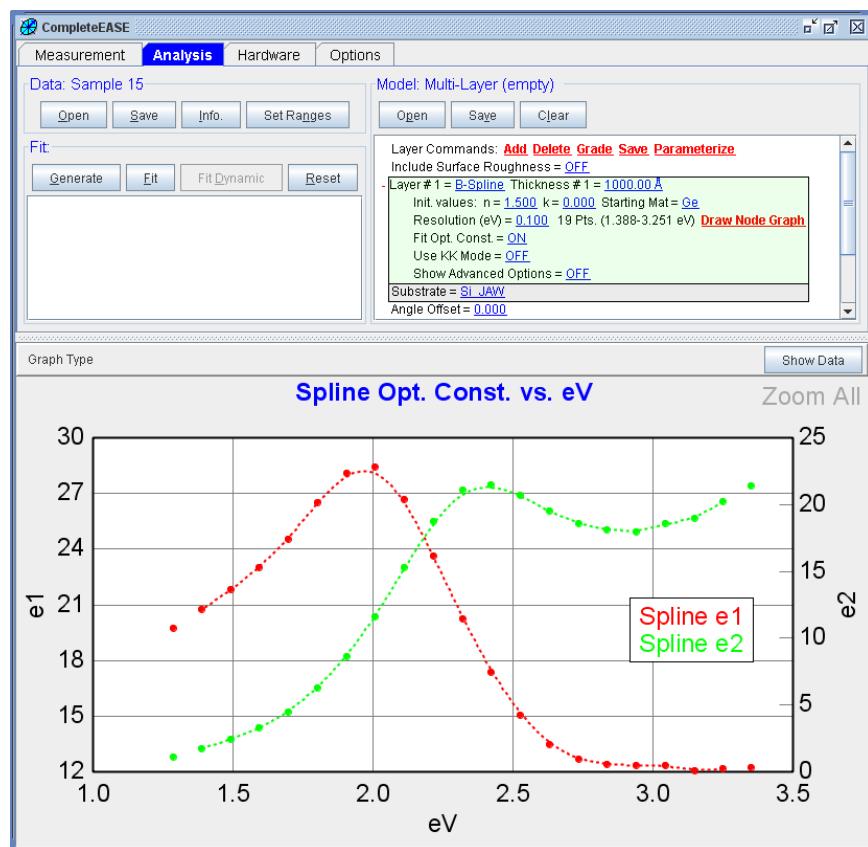


Figure 8-32. B-Spline layer and nodes matched to Germanium.

The B-Spline layer uses b-spline (also known as basis spline) curves to represent the dielectric function ( $\epsilon_1$  and  $\epsilon_2$ ) vs. eV. B-spline curves are defined by a series nodes (or “knots”), which have a position and amplitude. Basis polynomial functions at each node are defined by the recursive B-spline formula (Cheney and Kincaid, “Numerical Mathematics and Computing,” Third Edition, Brooks/Cole Publishing Company, 1994) in terms of the positions of the adjacent nodes. Summing the basis functions (weighted by the amplitude at each node) produces the resulting curve. B-spline curves have many desirable properties for modeling dielectric functions:

- b-spline curves and their derivatives (up to the spline order minus one) are continuous (the B-Spline layer uses 3rd order b-splines)
- the b-spline node amplitudes affect only the “local” shape of the curve, e.g., changing a node amplitude in the UV does not affect the curve in the VIS
- b-spline curves exhibit a “convex hull” property, e.g., if all the node amplitudes are non-negative, then the b-spline curve is also non-negative, thus avoiding non-physical negative  $\epsilon_2$  values
- since the basis functions depend only on the node positions, the node amplitudes which define the resulting curve are linearly independent, which greatly increases computation efficiency
- the Kramers-Kronig (K-K) integral can be applied to the b-spline recursion formula to generate K-K consistent basis functions (i.e., the  $\epsilon_1$  curve is defined by the K-K transform of  $\epsilon_2$ )

Figure 8-33 shows the default settings for the CompleteEASE B-Spline layer. The node amplitudes can be initialized to constant n and k values (vs. eV) by clicking on the “n=” or “k=” fields, or they can be initialized by specifying a “Starting Mat”. The “Resolution (eV)” field defines the nominal spacing of the nodes, which are equally distributed in eV over the selected spectral range of the data set. Clicking the “Draw Node Graph” field plots the positions and amplitudes of the b-spline nodes, along with the calculated dielectric function of the layer (Figure 8-34). The “Fit Opt. Const.” setting turns ON and OFF all the optical constant fitting parameters for the layer (e.g., node amplitudes and positions, pole amplitudes, etc.). If “Use KK Mode = OFF”, separate b-spline curves are calculated and fit for  $\epsilon_1$  and  $\epsilon_2$ . When “Use KK Mode = ON”, a b-spline curve is used to define  $\epsilon_2$ , and  $\epsilon_1$  is calculated from via the K-K transform of  $\epsilon_2$  (plus contributions from absorption outside the measured spectral range). Figure 8-35 shows the Node positions when KK Mode is turned on. Notice, there are nodes to describe  $\epsilon_2$ , along with a few nodes outside the measured spectral range – to help with the Kramers-Kronig integration.

The B-Spline layer will automatically extrapolate/interpolate/seed node amplitudes and positions if the selected spectral range and/or resolution is changed, or if KK Mode is toggled.

- Substrate = [B-Spline](#)  
 Init. values: n = [1.500](#) k = [0.000](#) Starting Mat = [none](#)  
 Resolution (eV) = [0.300](#) 6 Pts. (1.379-3.177 eV) [Draw Node Graph](#)  
 Fit Opt. Const. = [ON](#)  
 Use KK Mode = [OFF](#)  
[Show Advanced Options](#) = [OFF](#)

Figure 8-33. Default settings for the B-Spline layer.

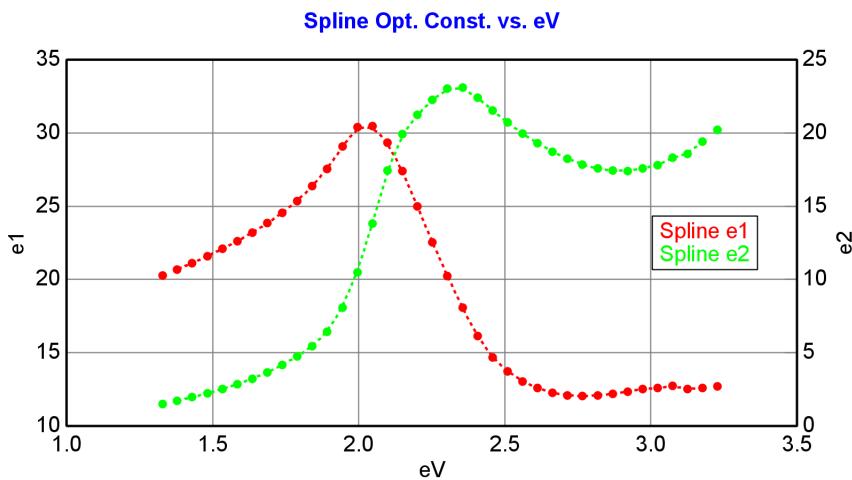


Figure 8-34. B-Spline layer Node Graph with KK Mode = OFF

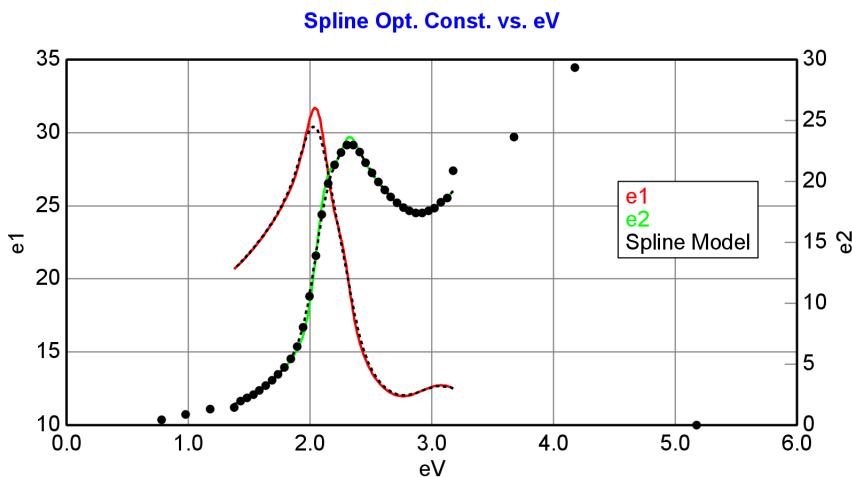


Figure 8-35. B-Spline layer Node Graph with KK Mode = ON.

All the available options for the B-Spline layer are shown in Figure 8-36. A brief description of each option follows:

**E Inf:** This stand for  $\epsilon_1$  and infinity, and when in KK mode it accounts for the absorption far outside the measured spectral range by adding a constant offset to the  $\epsilon_1$  curve.

**IR Amp:** With KK mode = ON, this value is the amplitude of a zero energy oscillator which accounts for absorption at low energies, typically due to free electron absorption (i.e., a Drude term).

**IR Br:** The broadening of the IR oscillator; often this can be fixed at zero, but allowing to vary can improve the fit to some metallic dielectric functions.

**Show Params:** Enables display of the all node amplitude fit parameters in the Fit Results; by default they are hidden to reduce the number of displayed parameters.

**Force E2 Positive:** Setting this to ON prevents  $\epsilon_2$  values from going negative. While this does enforce physicality to the dielectric function, sometimes allowing slightly negative  $\epsilon_2$  values improves the fit convergence.

**Assume Transparent Region:** A bandgap or spectral region can be specified for which  $\epsilon_2$  is fixed at zero.

**Use Default TieOff Behavior:** “TieOffs” are the nodes which account for absorption outside the spectral range when in KK mode. The “default” behavior (which specifies default TieOff node positions, and which amplitudes are fit for) is adequate for most applications. Turning the Default TieOff Behavior = OFF allows for complete flexibility in the TieOff positions and amplitudes.

**Tie Off Positions:** The positions and amplitudes of the Tie Offs can be set and defined as fit parameters. The positions are defined relative to the ends of the spectral range, and relative to each other to guarantee monotonically increasing node positions. Five node positions are defined above and below the spectral range; the amplitudes of the first and last two nodes are fixed at zero, while the other six node amplitudes can be fit.

```
- Substrate = B-Spline
  Init. values: n = 1.500 k = 0.000 Starting Mat = Ge
  Resolution (eV) = 0.050 36 Pts. (1.379-3.177 eV) Draw Node Graph
  E Inf = 0.657 (fit)
  IR Amp = -0.138 (fit) IR Br = 0.0000
  Fit Opt. Const. = ON
  Use KK Mode = ON (In Use)
  Show Advanced Options = ON
    ShowParms = OFF
    Force E2 Positive = OFF
    PreFit when changing wavelengths = ON
    Assume Transparent Region = ON
    Assume Band Gap = ON Band Gap (eV) = 1.200
    Use Default TieOff Behavior = ON
    View Tie Off Positions = ON
    Tie Off 0 {TieOff(1)-E} = 0.2000
    Tie Off 1 {TieOff(2)-E} = 0.2000
    Tie Off 2 {TieOff(3)-E} = 0.2000 spline_e2(0.779) = 0.0000
    Tie Off 3 {TieOff(4)-E} = 0.2000 spline_e2(0.979) = 0.0000
    Tie Off 4 (min-E) = 0.2000 spline_e2(1.179) = 0.0000
    Tie Off n+1 (max+E) = 0.5000 spline_e2(3.677) = 23.6615 (fit)
    Tie Off n+2 {TieOff(n+1)+E} = 0.5000 spline_e2(4.177) = 29.3344 (fit)
    Tie Off n+3 {TieOff(n+2)+E} = 1.0000 spline_e2(5.177) = 0.0000
    Tie Off n+4 {TieOff(n+3)+E} = 2.0000
    Tie Off n+5 {TieOff(n+4)+E} = 4.0000
```

Figure 8-36. B-Spline layer with all advanced options displayed.

## Intermix

If you add a layer and choose “Intermix” layer type before selecting where to add the layer (Figure 8-37), a special “Intermix” layer will be added that mixes the optical constants from the layer below and above in a 50-50% ratio. An example of this layer is shown in Figure 8-38. The intermix layer “steals” thickness away from the layer above and below to avoid moving the interference oscillations.

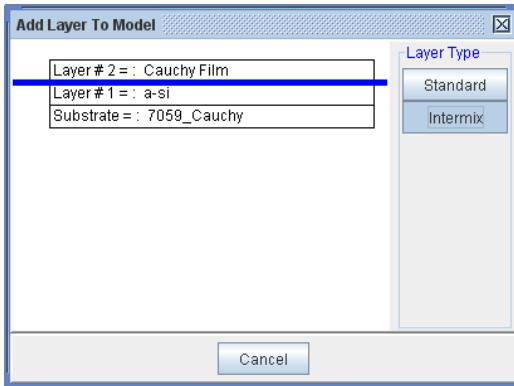


Figure 8-37. Choose “Intermix” before adding a layer between two layers to create a special layer that mixes the optical constants of the layers above and below wherever this layer is inserted.

|  |
|--|
| Layer # 2 = <u>SiO2</u> Thickness # 2 = <u>100.00 nm</u> |
| Intermix Thickness = <u>25.00 nm</u>                     |
| Layer # 1 = <u>a-si</u> Thickness # 1 = <u>50.00 nm</u>  |
| Substrate = <u>SI_JAW</u>                                |

Figure 8-38. Example of Intermix layer in a model.

## Composition Library

Layers that are marked as “Comp Library” or “Comp & Temp Library” are created to show variation in optical constants as the composition or temperature are varied.

Several of the material files provided with the CompleteEASE™ program contain information on the optical constants of a material as a function of temperature and/or alloy fraction. One example of this type of material is Al<sub>x</sub>Ga<sub>1-x</sub>As. The file AlGaAs\_T.MAT supplied with the CompleteEASE™ software contains information on the optical constants of Al<sub>x</sub>Ga<sub>1-x</sub>As over x values from 0 to 1 and temperature values from 577°C to 650°C. Using this type of layer is very similar to using the standard layer type for a material, the only difference being that there are temperature and/or alloy parameters that can be edited and fit for. Figure 8-39 shows how such a layer is represented in the model.

|   |
|---|
| - Substrate = <u>AlGaAs (Comp &amp; Temp Library)</u> |
| Composition = <u>0.20000</u>                          |
| Temperature = <u>500.00°C</u>                         |

Figure 8-39. A Temperature/Alloy layer as displayed in the model. The composition and temperature values are editable fit parameters.

## Coupled

Layer that has same optical constants as another layer in the model. An example is shown in Figure 8-40

|   |
|---|
| - Layer # 3 = <u>Coupled</u> Thickness # 3 = <u>200.00 nm</u> |
| Coupled to Layer # = <u>1</u> (Cauchy)                        |
| + Layer # 2 = <u>Gen-Osc</u> Thickness # 2 = <u>50.00 nm</u>  |
| + Layer # 1 = <u>Cauchy</u> Thickness # 1 = <u>200.00 nm</u>  |
| Substrate = <u>Si</u>   |

Figure 8-40. The “Coupled” layer gets optical constants from another layer in the model. In this case, it is using the optical constants from Layer #1, the Cauchy.

## Uniaxial and Uniaxial-Diff

Layers used to describe anisotropic materials. The Uniaxial layer is shown in Figure 8-41. Enter any material file into the Ordinary OC (in-plane optical constants) and Extra-Ordinary OC (out-of-plane optical constants) sections. In this example, Cauchy dispersions were used. The Uniaxial-Diff layer is similar, but you only enter a material file for the Ordinary optical constants. The remaining terms are used to express the index difference in a Cauchy-like summation to determine the Extra-ordinary optical constants. An example of the Uniaxial-Diff layer is shown in Figure 8-42.

|  |
|--|
| - Substrate = <u>Uniaxial</u>                                      |
| - Ordinary OC = <u>Cauchy</u>                                      |
| A = <u>1.450</u> (fit) B = <u>0.01000</u> (fit) C = <u>0.00000</u> |
| k Amplitude = <u>0.00000</u> Exponent = <u>1.500</u>               |
| Band Edge = <u>400.0 nm</u>  |
| - Extra-Ordinary OC = <u>Cauchy</u>                                |
| A = <u>1.550</u> (fit) B = <u>0.01000</u> (fit) C = <u>0.00000</u> |
| k Amplitude = <u>0.00000</u> Exponent = <u>1.500</u>               |
| Band Edge = <u>400.0 nm</u>  |

Figure 8-41. Example of the Uniaxial layer. Enter any material file for both the ordinary (in-plane) and extraordinary (out-of-plane) optical constants.

|  |
|--|
| - Substrate = <u>Uniaxial-Diff</u>                     |
| - Ordinary OC = <u>Cauchy_Wvl</u>                      |
| n = <u>1.450</u> B = <u>0.01000</u> C = <u>0.00000</u> |
| Design wvl = <u>632.8 nm</u>                           |
| A = <u>0.10000</u>                                     |
| B = <u>0.00000</u>                                     |
| C = <u>0.00000</u>                                     |
| D = <u>0.00000</u>                                     |

Figure 8-42. Example of the Uniaxial-Diff layer. Enter any material file for the ordinary (in-plane) optical constants and then use the 4-parameter dispersion (Cauchy-like) to describe the index difference..

---

## 8.6. Gen-Osc Oscillator Details

### e1 Offset

Purely real constant added to  $\varepsilon_l$ . It is equivalent to “ $\varepsilon_\infty$ ”, which is often seen in scientific literature.

### Pole

Poles describe zero-broadening oscillators. As such, they only affect the real part of the dielectric function ( $\varepsilon_l$ ). They can describe dispersion created by absorptions that occur **outside** the measured spectral range. They are defined in the equation:

$$\varepsilon_{n\_pole} = \frac{A_n}{E_n^2 - E^2}$$

### Lorentz

This is the classic Lorentz oscillator model, described as:

$$\varepsilon = \sum_{j=Osc\#} \left( \frac{(A_j + iZ_j)B_jC_j}{C_j^2 - \lambda^2 - iB_j\lambda} \right) + \varepsilon_\infty$$

### Harmonic

This is the classic Harmonic oscillator model. When the broadening becomes much less than the center energy (Brn,<<En), a Harmonic oscillator behaves as a Lorentz oscillator. The equation is described as:

$$\varepsilon = \sum_{j=Osc\#} \left( (A_j + iZ_j) \frac{1}{2} B \left( \frac{1}{C_j - \lambda - i(\frac{1}{2}B_j)} + \frac{1}{C_j + \lambda - i(\frac{1}{2}B_j)} \right) \right) + \varepsilon_\infty$$

### Gaussian

This Oscillator type produces a Gaussian line shape in  $\varepsilon_2$  with a Kramers-Kronig consistent line shape for  $\varepsilon_l$ .

$$\varepsilon_l = \varepsilon_\infty + \sum_{i=Osc\#} \left( A_i \left( \Gamma \left( \frac{\lambda - C}{k_G B} \right) + \Gamma \left( \frac{\lambda + C}{k_G B} \right) \right) + Z_i \left( \exp \left( - \left( \frac{\lambda - C}{k_G B} \right)^2 \right) + \exp \left( - \left( \frac{\lambda + C}{k_G B} \right)^2 \right) \right) \right)$$

$$\varepsilon_2 = \sum_i \left( A_i \left( \exp \left( - \left( \frac{\lambda - C}{k_G B} \right)^2 \right) + \exp \left( - \left( \frac{\lambda + C}{k_G B} \right)^2 \right) \right) + Z_i \left( \Gamma \left( \frac{\lambda - C}{k_G B} \right) + \Gamma \left( \frac{\lambda + C}{k_G B} \right) \right) \right)$$

where  $A$  is the real part of the amplitude,  $Z$  is the imaginary part of the amplitude,  $B$  is the broadening, and  $C$  is the center energy. The constant  $k_G$  is 0.600561294, and  $\lambda$  is the photon energy in eV. The function  $\Gamma$  is a convergence series.

The oscillators in this layer are defined so that the amplitude is the height of the oscillator's  $\varepsilon_2$  peak at its center energy and the broadening is the full width of the oscillator at half maximum value (FWHM). This way, when an oscillator's type is changed, the new oscillator has the same height and FWHM as the old oscillator.

## Drude

The classic Drude model describes free carrier effects on the dielectric response. Its form is a Lorentz oscillator with zero resonance energy. The Drude dispersion type is described in the equation below. It is defined in terms of the dc resistivity ( $\rho$ ) and mean scattering time ( $\tau$ ). The units of  $\rho$  are  $\Omega\text{cm}$  and the units of  $\tau$  are femtoseconds.

$$\tilde{\epsilon}(\lambda) = \epsilon_{\infty} - \frac{i4\pi\hbar^2}{\rho(\hbar\lambda + i\lambda^2\tau)}$$

## Tauc-Lorentz and Cody-Lorentz

The Tauc-Lorentz and Cody-Lorentz dispersion types are primarily designed for modeling amorphous materials. The main difference between the two types is how they model absorption at energies slightly larger than the energy gap. In this region the Tauc-Lorentz model follows the Tauc law formula while the Cody-Lorentz follows the Cody formula:

*Tauc Absorption Formula:*  $\epsilon_2(E) \propto [(E - Eg)^2/E^2]$

*Cody Absorption Formula:*  $\epsilon_2(E) \propto (E - Eg)^2$

The Cody-Lorentz type also includes an Urbach absorption term. The fit parameters for the Tauc Lorentz are the Amplitude (Amp), Broadening (Br), Center Energy (Eo), and Band Gap (Eg). The Cody-Lorentz oscillator adds Ep (transition energy where absorption changes from Lorentzian to Cody), and Et (transition energy where absorption changes from Cody behavior to Urbach behavior). Figure 8-43 shows how the Ep and Et are defined.

The *Tauc-Lorentz* oscillator term was developed by Jellison and Modine<sup>5</sup>. It works particularly well for amorphous materials.

The Cody-Lorentz oscillator model, which was developed by Ferlauto, et al<sup>6</sup>, is also designed for amorphous materials. It is similar to the Tauc-Lorentz in that it defines a bandgap energy, Eg, and a Lorentzian absorption peak (parameters Amp, En, and Br). However, the two models behave quite differently in the absorption-onset region, at photon energies slightly greater than Eg. In that region, the Tauc-Lorentz model follows a Tauc law formula,  $\epsilon_2(E) \propto [(E - Eg)^2/E^2]$ , while Cody-Lorentz model assumes that  $\epsilon_2(E) \propto (E - Eg)^2$ . The model also includes an Urbach absorption term.

<sup>5</sup> G.E. Jellison, Jr. and F.A. Modine, “Parameterization of the optical functions of amorphous materials in the interband region,” Appl. Phys. Lett. **69**, 371 (1996), Erratum, Appl. Phys. Lett. **69**, 2137 (1996).

<sup>6</sup> A.S. Ferlauto, G.M Ferreira, J.M. Pearce, C.R. Wronski, R.W. Collins, Xunming Deng, and Gautam Ganguly, “Analytical model for the optical functions of amorphous semiconductors from the near-infrared to ultraviolet: Applications in thin film photovoltaics,” J. Appl. Phys. **92**, 2424 (2002).

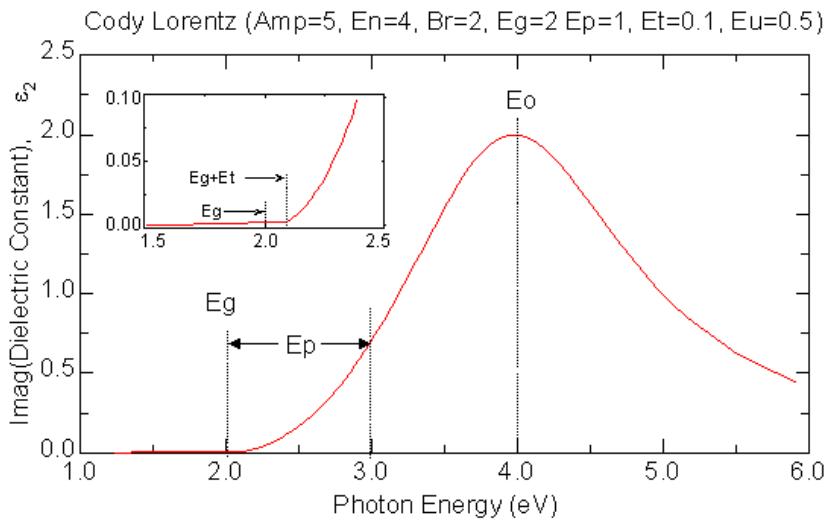


Figure 8-43. Parameter definitions for the Cody-Lorentz oscillator in Gen-Osc.

## 8.7. +MODEL Options

The full list of +MODEL Options are shown in Figure 8-44. To view many of these, you first need to select [Configure Options](#).

- **MODEL Options**
  - Include Substrate Backside Correction = [OFF](#)
  - Model Calculation = [Ideal](#)
  - Ambient Index >1 = [OFF](#)
  - Wvl. Shift (nm) = [0.00](#)
  - Return Path Ellipsometer = [OFF](#)
  - Delta Offset: [None](#)
  - Source Rot. = [0.000](#) Receiver Rot. = [0.000](#)
- Multi Sample Analysis**
  - [Add Fit Parameter](#) [Delete All Params](#)
  - [Data Set](#)

Figure 8-44. List of all +MODEL Options

### Include Substrate Backside Correction

Calculate the incoherent contribution of light reflecting from backside of transparent substrates in the model.

### Model Calculation

Choose different model calculations (Figure 8-45) to handle non-ideal sample situations. For most samples, the default setting of “Ideal” is preferred. However, there are choices to “Include Bandwidth (eV)”, “Include Thickness Nonuniformity”, and “Include Bandwidth(nm)”, when these non-ideal situations are suspected. These options are best used in conjunction with Depolarization data fitting.

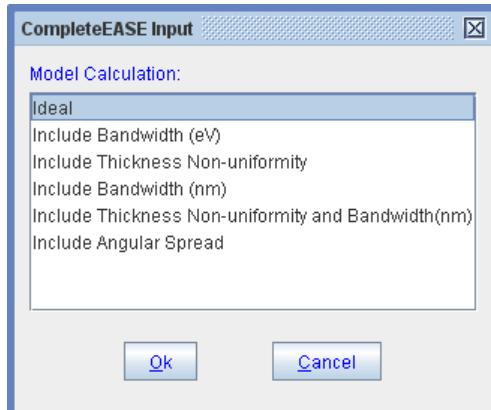


Figure 8-45. Different model calculation types.

### **Ambient Index > 1**

Use when working with liquid-cell where ambient is water or some other solution.

### **Wvl Shift (nm)**

Use to simulate a wavelength shift.

### **Return Path Ellipsometer**

Special configuration of M-2000 where source and detector are mounted side-by-side and the measurement beam reflects from the sample, then from a mirror and back off the sample surface on the way back to ellipsometer.

### **Delta Offset**

Used to correct for windows.

### **Source and Receive Rot.**

Enter for rotation of the source or receiver.

### **Multi-Sample Analysis**

When multiple data sets are appended, but from different samples, they can be fit simultaneously and this section allows different fit parameters to have multiple “values”. An example of multi-sample analysis is shown in Figure 8-46, where three oxides on silicon are fit with a common Cauchy layer to describe same index, but the thicknesses are allowed to differ for each data set.

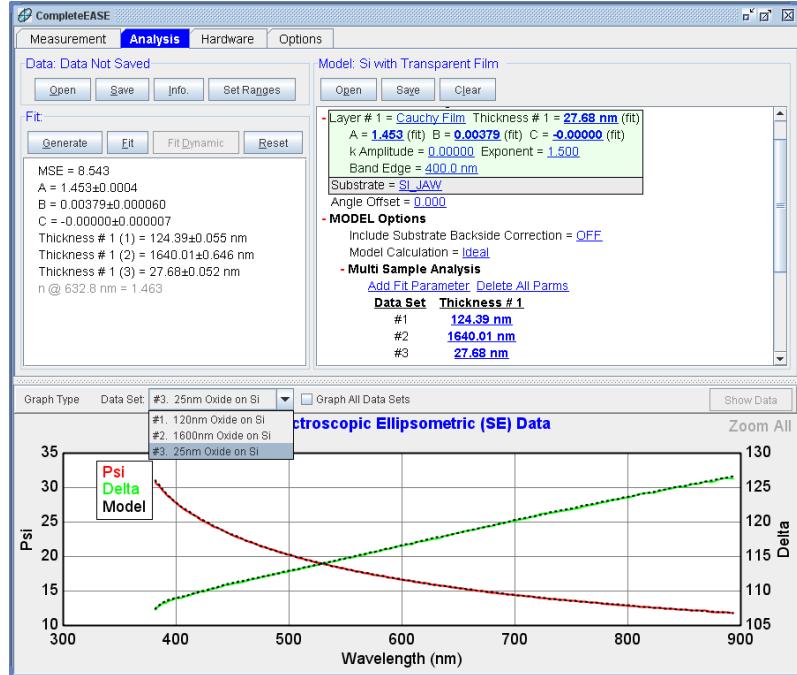


Figure 8-46. Example of Multi-Sample Analysis, where all three data sets are fit simultaneously with common Cauchy optical constants and different film thickness.

## 8.8. +FIT Options

The full list of **+FIT Options** are shown in Figure 8-47. To view many of these, you first need to select [Configure Options](#).

- **FIT Options**
  - Perform Thickness Pre-Fit = [OFF](#)
  - Use Global Fit = [ON](#)
    - # of Data Points = [100](#) # of Iterations = [5](#)
    - Parm #1 = [Thickness #1](#)
      - Min. = [0.00 nm](#) Max. = [1000.00 nm](#) # Guesses = [50](#)
      - Parm #2 = [\(none\)](#)
      - Parm #3 = [\(none\)](#)
    - Include Wvl. Range Expansion Fits = [OFF](#)
  - Selected Data = [Standard Ellipsometric](#)
  - Fit Weight = [N.C.S](#)
  - Include Depolarization Data = [ON](#) % Weight = [100.00](#)
  - Include Intensity Data = [ON](#) % Weight = [100.00](#)
  - Transmission Data % Weight = [100.00](#)
  - Limit Wvl. for Fit = [ON](#) Range = [370.0 nm - 5000.0 nm](#)
  - Skip Data Points in Fit = [0](#)
  - Include Derived Parameters = [ON](#)
    - [Add Derived Parameter](#)
    - 1: Type = [n](#) Layer # = [1](#) Wavelength = [632.8 nm](#) Name : [Low Spec. = 0.000 High Spec. = 0.000](#)

Figure 8-47. List of all **+FIT Options**.

## Perform Thickness Pre-Fit

When turned on, it uses a patent-pending algorithm to quickly estimate the thickness for the thickest layer in the model.

## Use Global Fit

Allows fit parameters to be varied over a range of values to find the best match to the data. The Global Fit is described in detail in the Example of Section 3.3.

### ***Number of Data Points to Use***

Used by Global Fit to improve speed. This refers to the number of wavelengths used during the Global search.

### ***Number of Global Fit Iterations***

This is the number of guesses to search over.

### ***Parm. #1, #2, #3***

Up to three fit parameters can be included in the Global Fit.

### ***Min. / Max. and # Guesses***

Select the “search” range for each Fit Parameter that is included in the Global Search, along with the number of guesses between the minimum and maximum values.

### ***Include Wvl. Expansion Fits***

Decide whether the Global Fit should also use the Wvl Expansion Fit

### ***Limit Wvl for Fit***

Select a limited spectral range during the fit to increase speed of the Global Fit..

## Selected Data

Choose which type of data to include in the Fit. Choices include Standard Ellipsometry (SE), generalized-SE, Mueller-matrix, and Intensity data only, as shown in Figure 8-48.

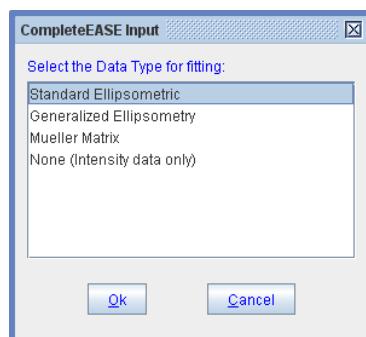


Figure 8-48. Choose the selected data type to use during fit.

## Fit Weight

Select the fit weighting, with choices as shown in Figure 8-49.

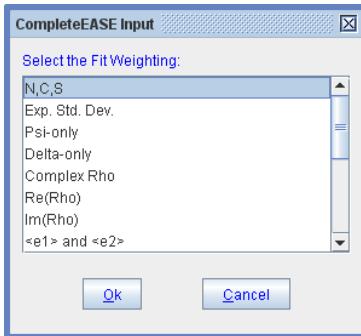


Figure 8-49. Select the Fit Weighting.

## Include Depolarization Data

Turn this setting on when you want the depolarization data to be included as part of the fit weighting.

## Include Intensity Data

Choose whether intensity data should be included in the fit weighting, turn on this setting.

## Transmission Data % Weight

When Transmission Intensity data is fit along with SE data, it is default to equal weighting in the fit (100%). This setting allows more or less importance to be placed on the Transmission Intensity data by increasing or reducing this percentage, respectively.

## Limit Wvl. for Fit

Reduce the wavelength used during fitting.

## Skip Data Points in the Fit

Reduce the number of wavelength used during fitting by skipping this number of points.

## Include Derived Parameters

To add a derived parameter to a model, open the Fit Options section and then turn the “Include Derived Parameters” flag to “ON”. This allows you to add multiple derived parameters. Figure 8-50 below shows how a derived parameter for displaying the index of refraction at 632nm would look.

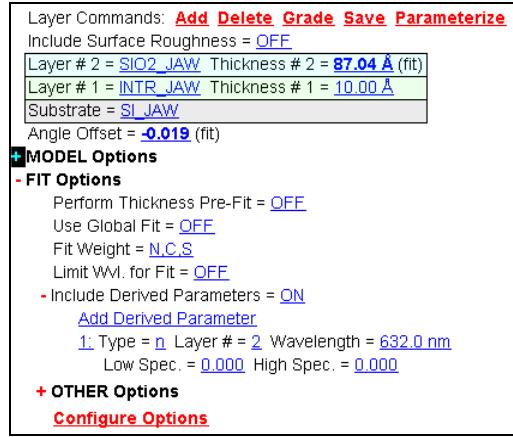


Figure 8-50. Derived Parameters in +FIT Options

Clicking the mouse on the Type parameter allows you to change the derived parameter calculation. The available types are shown in Figure 8-51. Some of the types allow the specification of a wavelength and layer number for the parameter.

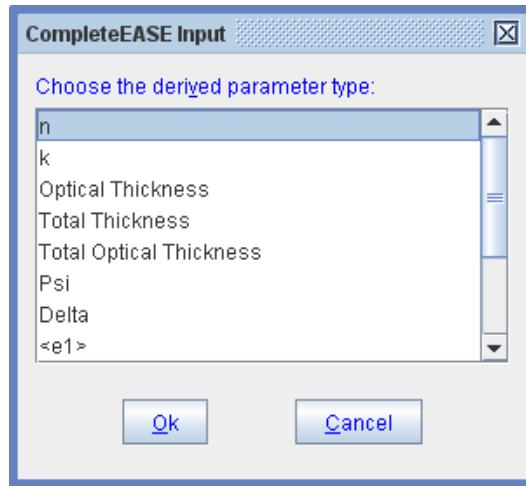


Figure 8-51. Derived Parameter Types.

After fitting data using a model with derived parameters, the fit results section shows the model fit parameters and the derived parameters. The derived parameters are shown in gray instead of black.

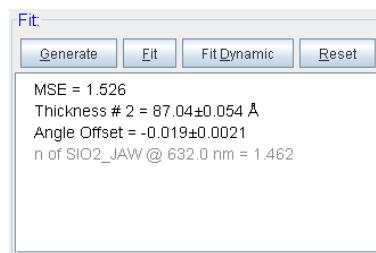


Figure 8-52. Fit Results window showing the Derived Parameter for index of the SiO2 layer at 632nm.

A new derived parameter type called “User Equation” has been added to CompleteEASE (new in version 3.38) so simple calculations can be performed after a fit has finished. If there is an error in the equation then the derived parameter will not be displayed in the **Fit** section after a fit is completed. This derived parameter has 4 items that can be edited – a name, equation, and low and high specifications. Figure 8-53 shows how the derived parameter displays in a model.

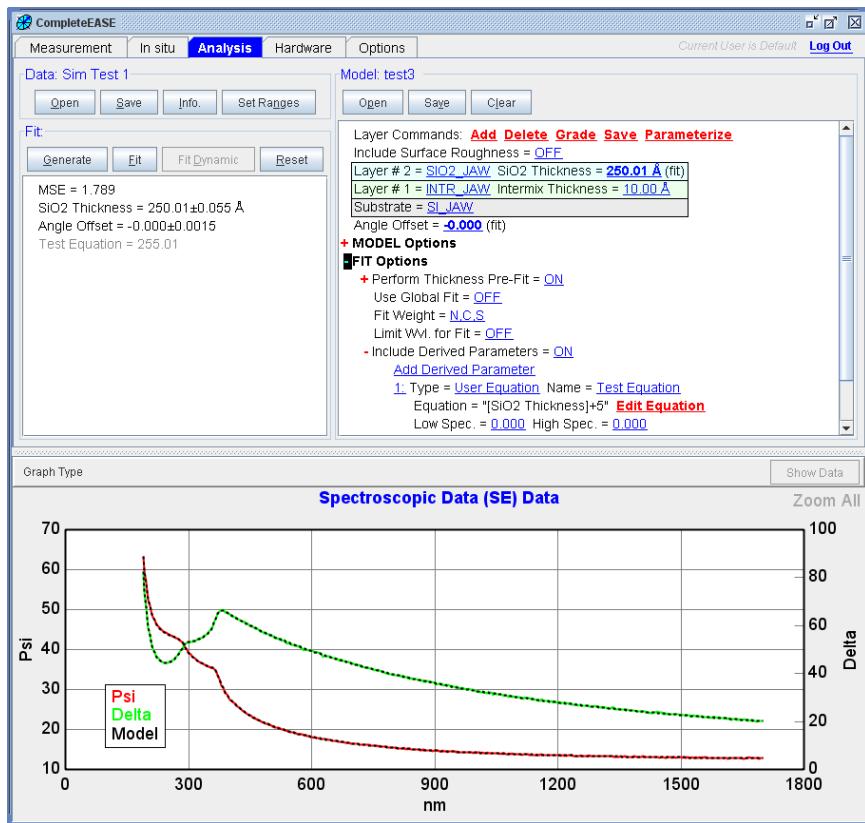


Figure 8-53. Display of the Add Derived Parameter within the model.

To edit the equation press the **Edit Equation** item. This brings up the Edit Equation dialog as shown in Figure 8-54. In addition to specifying the equation this dialog allows the user to enter the number of decimal places that should be displayed.

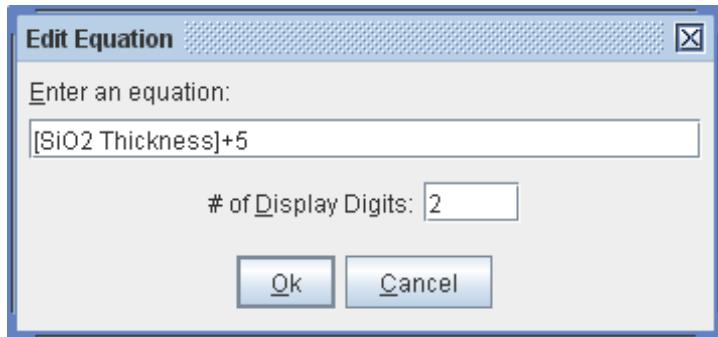


Figure 8-54. Edit Equation Dialog Box

The equation can contain numbers, operators, variables, and parentheses for grouping. The available operators are: ‘+’ (add), ‘-’ (subtract), ‘\*’ (multiply), ‘/’ (divide), and ‘^’ (power). In addition there are a number of constants and functions that can be used. These are shown below.

### ***Functions***

- sin
- cos
- tan
- log
- abs
- sqrt

### ***Constants***

- PI
- e

Variables in an equation are fit parameter names in enclosing brackets. An example would be “[SiO<sub>2</sub> Thickness]”. Any fit parameter name can be specified as well as any derived parameter names that appears in the list above the equation.

---

## **8.9. +OTHER Options**

### **Wvl. Range Expansion Fit**

Press this command to execute a Wavelength-Range Expansion Fit. The model is restricted to longer wavelengths and fit. Then, the data range is increased toward shorter wavelengths in increments. As each new range of data is added, the data are fit again. This method works well in combination with the B-Spline layer and is demonstrated in Example of Section 4.3

### **Try Alternate Models**

The “Try Alternate Models” command automatically fits the data using the ideal layered optical model, and then with surface roughness and index grading non-idealities added to the model. The results of the various model fits are summarized in tabulated and graphical format, and the user can then decide which model is most appropriate for the sample. Example of report generated by this command is shown in Figure 8-55.

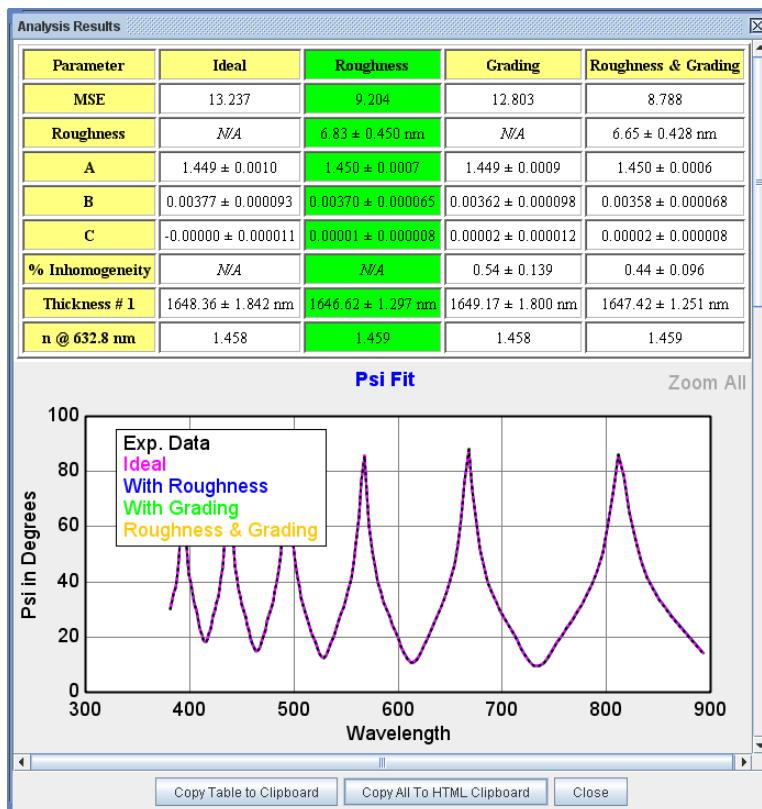


Figure 8-55. Example of the Try Alternate Models report that is generated.

## Parameter Uniqueness

This command allows user to test the uniqueness of a fit parameter. A single fit parameter is selected to vary over a range of values. At each value, the fit parameter is fixed while all other fit parameters are varied to find the best fit (lowest MSE). The MSE is recorded to visualize the shape of MSE profile versus the varied fit parameter. An example MSE profile is shown in Figure 8-56.

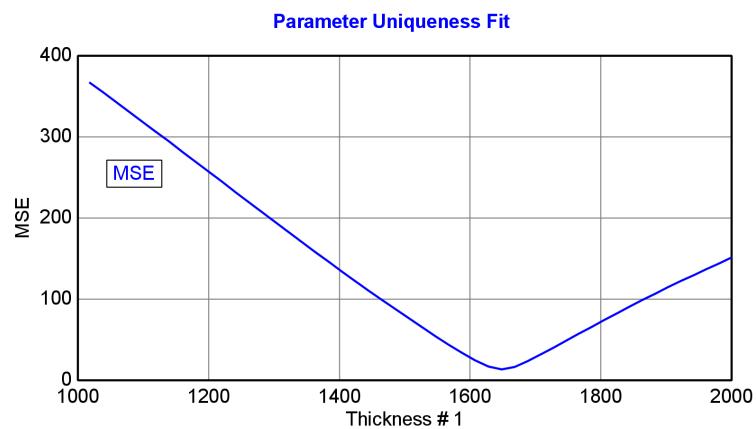


Figure 8-56. MSE profile from Parameter Uniqueness test.

## **Simulate Data**

This option is used to simulate data based on the existing model. When the command is pressed, you will see the simulation settings as listed in Figure 8-57.

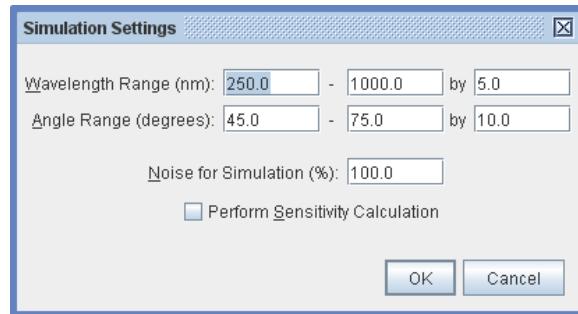


Figure 8-57. Simulation Settings.

## **Add Opt. Const. to HTML Report**

Choose this option to automatically add optical constants graphs to the HTML report.

## **Configure Options**

Choose this command to show “hidden” features in the **+MODEL Options**, **+FIT Options**, and **+OTHER Options** sections of the model. The choices are shown in Figure.

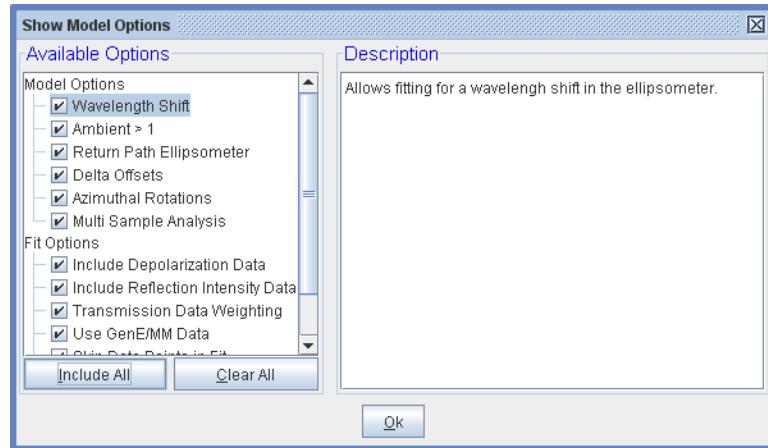


Figure 8-58. Configure which “hidden” options to show within the Model.

# 9. Reference - Hardware Tab

The controls available in the **Hardware** tab are different for the different ellipsometer configurations. As a result, this chapter is divided into two major sections: one section describing the AlphaSE's **Hardware** tab and another section describing the M-2000 and RC2 **Hardware** tab.

## 9.1. Hardware Tab – AlphaSE

The **Hardware** tab for an AlphaSE is shown in Figure 9-1. This tab consists of four panels: **Hardware**, **Signal**, **Calibration**, and **Show Logs**. A brief description of all commands within this tab is described.

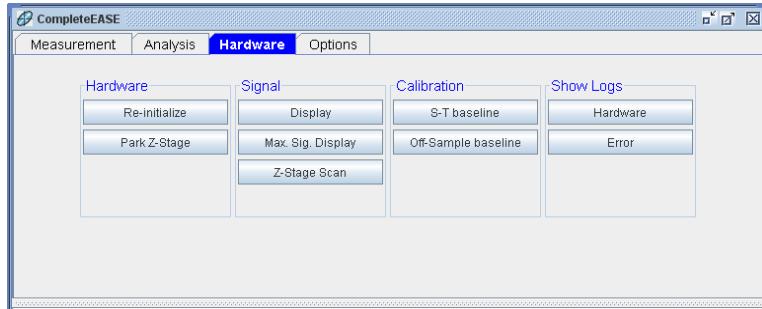


Figure 9-1. CompleteEASE software with the **Hardware** tab selected.

### Hardware

#### Re-initialize

This button re-initializes the ellipsometer hardware, which initiates communication over the USB link, scans the spectrometer, moves the motors to home position, and tests the motors. Details of any errors that occur during hardware initialization can be found in the “Hardware” and/or “Error” logs.

#### Park Z-Stage

Moves the Z-stage to the “park” position such that the Z-stage shipping lock can be engaged.

## Signal

### Display

Displays signal intensity of the light collected by the spectrometer. Average, maximum, UV, and IR intensity values are also reported in the status box, along with the current spectrometer “Dark Count” and electronics “Temperature”. An example is shown in Figure 9-2.

### Max. Sig. Display

Same as Display, except that the polarizer and compensator optics are adjusted to find the maximum signal intensity. Window will appear as shown in Figure 9-2, after the maximum signal is found.

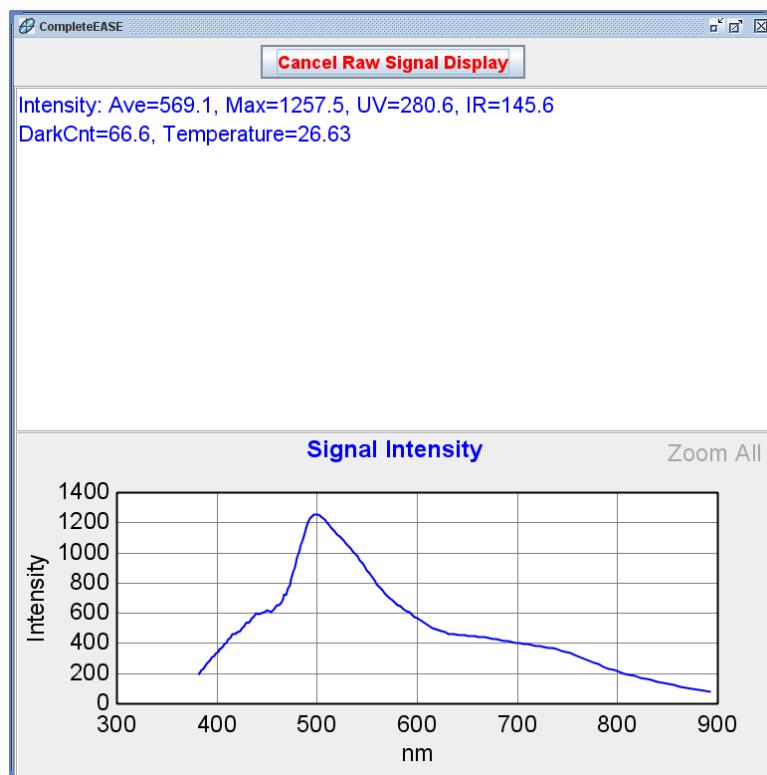


Figure 9-2. CompleteEASE “Signal Display” screen.

### Z-Stage Scan

Scans the Z-stage to generate intensity vs. sample height profile. A sample should be mounted and the ellipsometer unit set to the “Off-Sample” configuration before clicking this button. The resulting signal intensity profile should appear symmetrical, similar to the graph shown in Figure 9-3. The black dashed curve is a polynomial fit to the measured profile, and the reported “MSE=” value quantifies the symmetry of the profile. If the MSE value is greater than 0.02, contact your J.A. Woollam Co., Inc. representative.

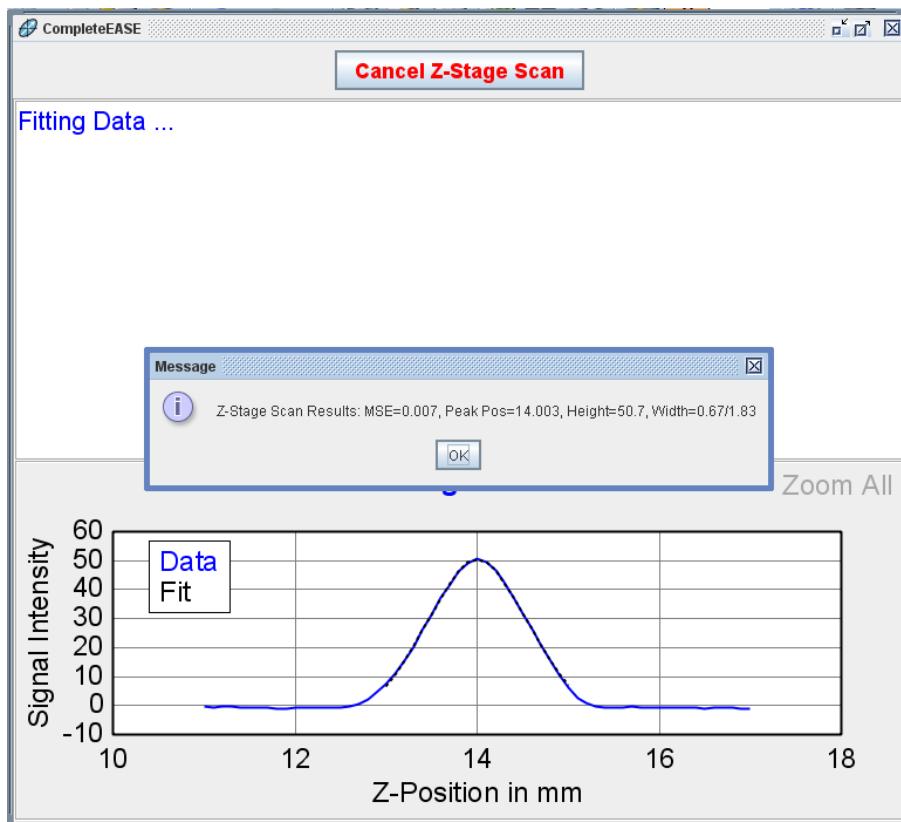


Figure 9-3. Results of a typical Z-Stage scan.

## Calibration

### S-T Baseline

Acquires baseline spectra for the “Straight-Through” configuration such that accurate transmission intensity and Mueller matrix data can be acquired. For best data accuracy, always perform a S-T Baseline after moving the ellipsometer optics, or if it has been a long time (> 1 hour) since the previous baseline.

### Off-Sample Baseline

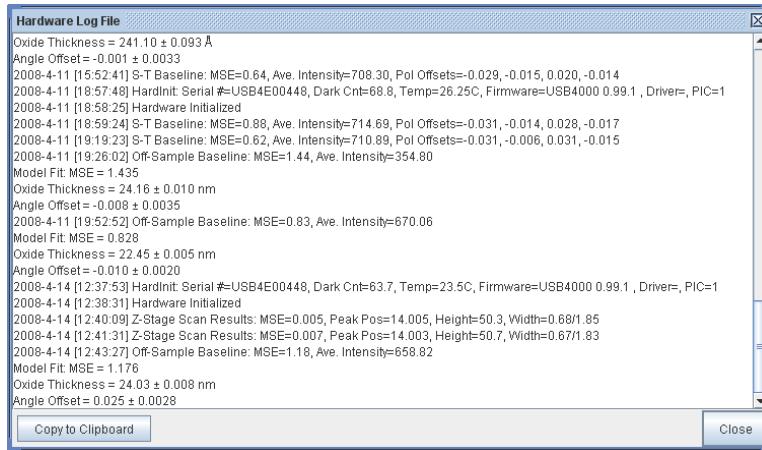
Acquires an “Off-Sample” baseline such that qualitative reflection intensity data can be acquired. This option also calibrates and stores the angle of incidence which is used for subsequent measurements. For best angle of incidence accuracy, perform an Off-Sample Baseline after moving the source or receiver units, or after mounting the sample chuck.

## Show Logs

### **Hardware and Error Logs**

These buttons display the Hardware and Error logs, which contain information useful for diagnosing and debugging problems with the instrument. If the instrument is not working properly, your J.A. Woollam Co., Inc. representative may require this

information to diagnose the problem: click the “Save Debug File” button that appears in the log file, and email C:\CompleteEASE\CompleteEASE\_Debug.zip file. An example Hardware Log is shown in Figure 9-4 and Error Log is shown in Figure 9-5.

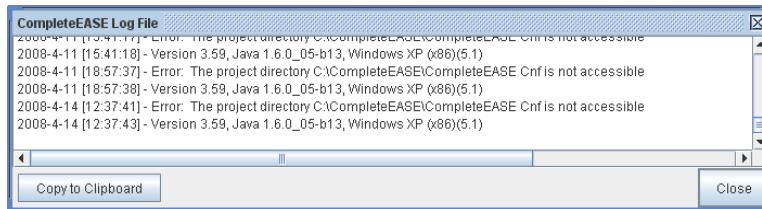


The screenshot shows a window titled "Hardware Log File". The log contains several entries related to oxide thickness measurements and hardware initialization. Key entries include:

- Oxide Thickness =  $241.10 \pm 0.093 \text{ \AA}$
- Angle Offset =  $-0.001 \pm 0.0033$
- 2008-4-11 [15:52:41] S-T Baseline: MSE=0.64, Ave. Intensity=708.30, Pol Offsets=-0.029, -0.015, 0.020, -0.014
- 2008-4-11 [18:57:48] HardInit Serial #:USB4E00448, Dark Cnt=68.8, Temp=26.25C, Firmware=USB4000 0.99.1 , Driver=, PIC=1
- 2008-4-11 [18:59:25] Hardware Initialized
- 2008-4-11 [18:59:24] S-T Baseline: MSE=0.88, Ave. Intensity=714.69, Pol Offsets=-0.031, -0.014, 0.028, -0.017
- 2008-4-11 [19:19:23] S-T Baseline: MSE=0.62, Ave. Intensity=710.89, Pol Offsets=-0.031, -0.006, 0.031, -0.015
- 2008-4-11 [19:26:02] Off-Sample Baseline: MSE=1.44, Ave. Intensity=354.80
- Model Fit: MSE = 1.435
- Oxide Thickness =  $24.16 \pm 0.010 \text{ nm}$
- Angle Offset =  $-0.008 \pm 0.0035$
- 2008-4-11 [19:52:52] Off-Sample Baseline: MSE=0.83, Ave. Intensity=670.06
- Model Fit: MSE = 0.828
- Oxide Thickness =  $22.45 \pm 0.005 \text{ nm}$
- Angle Offset =  $-0.010 \pm 0.0020$
- 2008-4-14 [12:37:53] HardInit Serial #:USB4E00448, Dark Cnt=63.7, Temp=23.5C, Firmware=USB4000 0.99.1 , Driver=, PIC=1
- 2008-4-14 [12:38:31] Hardware Initialized
- 2008-4-14 [12:40:09] Z-Stage Scan Results: MSE=0.005, Peak Pos=14.005, Height=50.3, Width=0.68/1.85
- 2008-4-14 [12:41:31] Z-Stage Scan Results: MSE=0.007, Peak Pos=14.003, Height=50.7, Width=0.67/1.83
- 2008-4-14 [12:43:27] Off-Sample Baseline: MSE=1.18, Ave. Intensity=658.82
- Model Fit: MSE = 1.176
- Oxide Thickness =  $24.03 \pm 0.008 \text{ nm}$
- Angle Offset =  $0.025 \pm 0.0028$

Buttons at the bottom include "Copy to Clipboard" and "Close".

Figure 9-4. Hardware Log.



The screenshot shows a window titled "CompleteEASE Log File". The log displays several error messages from different dates and times, all reporting that the project directory is not accessible. Key errors include:

- 2008-4-11 [15:41:17] - Error: The project directory C:\CompleteEASE\CompleteEASE Cnf is not accessible
- 2008-4-11 [15:41:18] - Version 3.59, Java 1.6.0\_05-b13, Windows XP (x86)(5.1)
- 2008-4-11 [18:57:37] - Error: The project directory C:\CompleteEASE\CompleteEASE Cnf is not accessible
- 2008-4-11 [18:57:38] - Version 3.59, Java 1.6.0\_05-b13, Windows XP (x86)(5.1)
- 2008-4-14 [12:37:41] - Error: The project directory C:\CompleteEASE\CompleteEASE Cnf is not accessible
- 2008-4-14 [12:37:43] - Version 3.59, Java 1.6.0\_05-b13, Windows XP (x86)(5.1)

Buttons at the bottom include "Copy to Clipboard" and "Close".

Figure 9-5. Error Log.

## 9.2. Hardware Tab – M-2000 and RC2

Figure 9-6 shows the **Hardware** Tab for an M-2000 System. This tab consists of three panels: **Hardware Status**, **System Information**, and **Controls**. This section describes these panels and the controls found on them.

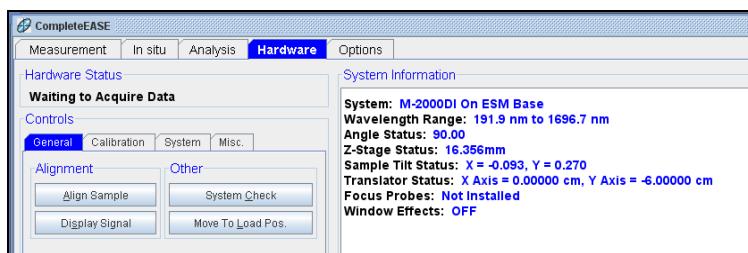


Figure 9-6. M-2000 and RC2 Hardware Tab.

## Hardware Status

The **Hardware Status** panel displays the current state of the hardware. This is the same information displayed in the **Hardware Status** panel of the **Measurement** tab.

## System Information

The **System Information** panel displays details about the ellipsometer configuration and provides access to the hardware configuration dialog and hardware log. The information provided includes the type of ellipsometer, wavelength range, and current motor positions. Please have this information available when contacting the J.A. Woollam Company for assistance.

### Edit Hardware Config.

Pressing this button will bring up the Hardware Configuration dialog. This dialog contains many settings for configuring the behaviour of the hardware. The dialog displays a description of each parameter's function so the items will not be described here.

### View Hardware Log

This button displays the Hardware log which contains information on calibrations and initializations.

## Controls

The **Controls** panel provides access to hardware functions other than those needed for acquiring data. The hardware functions are separated into groups displayed as tabs. The tabs are **General**, **Calibration**, **System**, and **Misc.**.

### General

The **General** tab shown in Figure 9-7 is nearly the same for all of the different ellipsometer configurations. The available controls are as follows:

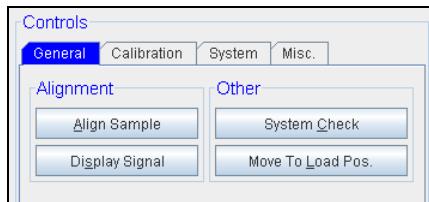


Figure 9-7. General Tab.

### Align Sample

Align the sample without acquiring data. For systems with automated alignment capabilities a dialog is displayed allowing the user to choose between manual alignment and automated alignment (Figure 9-8). Choosing No in the dialog displays the manual alignment dialog.



Figure 9-8. The Sample Alignment dialog gives the user a choice of automated alignment or manual alignment.

## Display Signal

This function displays the raw signal intensity. This screen is useful for debugging light intensity problems.

## System Check

A System Check is the most common procedure for calibrating the ellipsometer. See the hardware manual for details on the System Check procedure.

## Move To Load Pos.

This function configures the system to make loading a sample easier. This applies only to systems with automated z-stages and translators. Generally, pressing this button will result in the z-stage moving to its maximum value and the translator moving towards the user.

## Calibration

The **Calibration** tab appears different depending on the type of ellipsometer. Figure 9-9 shows the **Calibration** tab for an M-2000 and Figure 9-10 shows the tab for an RC2. It is not common for a user to need the controls in this tab as a System Check will perform many of these functions.

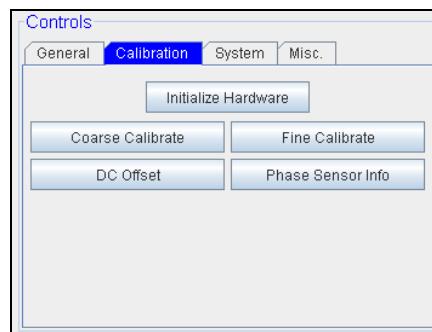


Figure 9-9. Calibration tab for M-2000 ellipsometers.

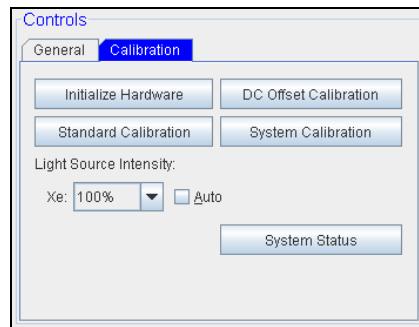


Figure 9-10. Calibration tab for RC2 ellipsometers.

## Initialize Hardware

This button re-initializes the ellipsometer hardware, which initiates communication over the USB/TCP/IP link, scans the spectrometer and moves the motors to home position. Details of any errors that occur during hardware initialization can be found in the “Error” log.

## Coarse Calibrate and Fine Calibrate (M-2000 Only)

These calibrations can be performed in place of a System Check when it is not possible to use the standard calibration wafer that is supplied with the instrument. This situation sometimes occurs during in situ measurements on a deposition chamber that requires a specific sample size. These calibrations will not determine the in-plane window effects. Always perform a System Check instead of a Coarse or Fine calibration when possible.

#### **DC Offset**

Measures the ambient light and electronic noise contribution to the measured raw intensity. This button is most often used before acquiring depolarization data to improve measurement accuracy. A System Check performs this measurement as well.

#### **Phase Sensor Info (M-2000 Only)**

This diagnostic function displays information used to determine if the phase sensor is working and the compensator motor is spinning. When troubleshooting a hardware problem a J.A. Woollam Company representative may ask for this information.

#### **Standard Calibration (RC2 Only)**

A Standard Calibration is equivalent to a Coarse Calibration on the M-2000. The System Check is the preferred method for calibrating the instrument when the standard calibration wafer can be used.

#### **System Calibration**

See the hardware manual for information on the System Calibration.

#### **Light Intensity (RC2 Only)**

The Light Intensity box allows the user to change the current light intensity. Normally this is left in automatic mode.

#### **System Status (RC2 Only)**

The System Status button displays a diagnostics dialog with information on the phase sensors and USB communication. When troubleshooting a hardware problem a J.A. Woollam Company representative may ask for this information.

### **System**

The controls in the **System** tab are dependent on the type of base the ellipsometer is attached to. The main types of bases are the ESM (horizontal sample mount, automated z-stage and angle), ES130 (horizontal sample mount, manual z-stage and angle), Fixed Angle Focused (horizontal sample mount, automated z-Stage), Vertical (vertical sample mount, automated angle), and Accumap. Some of the bases have multiple attachments which can also change the controls available on the System tab. Figure 9-11 through Figure 9-13 show the System tab for some of these bases. Brief descriptions of the different buttons on this panel can be found below. See the hardware manual for a detailed description of the use of these functions.

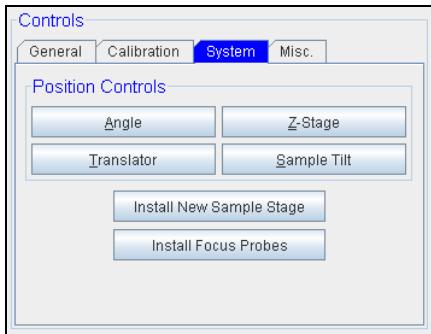


Figure 9-11. System tab for ESM, ES130, and Fixed Angle bases.

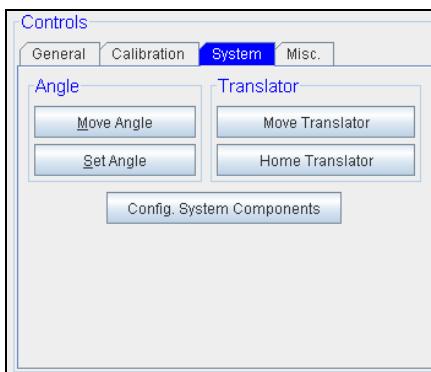


Figure 9-12. System tab for Vertical bases.

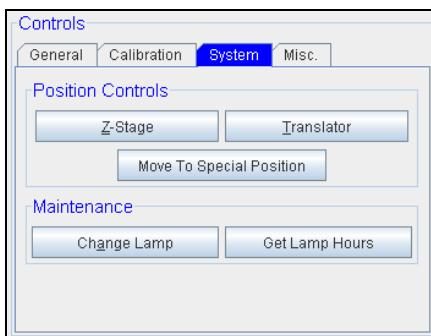


Figure 9-13. System tab for AccuMap systems.

### **Angle, Z-Stage, Translator, Sample Tilt**

These buttons allow the user to change the positions of the motorized base components. For example, to change the position of the Z-Stage, press the Z-Stage button and enter a position. The stage will then move to the specified position.

#### **Set Angle (Vertical base)**

The vertical sample-mount base does not have a home sensor for the angle so the Set Angle function allows the user to set the current angle.

#### **Install New Sample Stage (ESM, ES130 and Fixed Angle)**

This function steps the user through the process of installing a sample stage attachment. These attachments included items such as a Translator, Heat Cell, Liquid Cell, etc. On bases with automatic detection capabilities the software will

automatically detect which stage is being installed. The other bases will display a dialog with the different stage options and the user will select the one being installed.

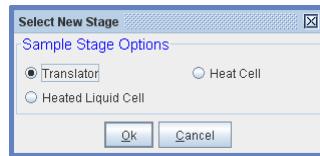


Figure 9-14. The Select New Stage dialog.

#### **Install/Remove Focus Probes (ESM, ES130 and Fixed Angle Focused)**

Steps the user through the focus probe installation/removal procedure.

#### **Configure System Components (Vertical base)**

This button displays a dialog that allows the user to specify the attachments that are currently installed. These attachments can include a translator, focus probes, camera, rotator, etc.

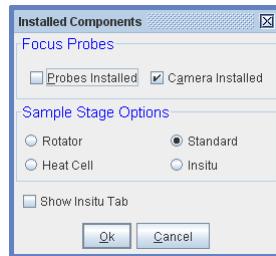


Figure 9-15. The Installed Components dialog for vertical bases.

#### **Change Lamp (AccuMap)**

Steps the user through the lamp change procedure. See the hardware manual for a description of this procedure.

#### **Get Lamp Hours (AccuMap)**

Displays the number of hours the lamp has been on since it was installed.

#### **Misc.**

The controls in the **Misc.** tab cover functions that did not fit into the **General**, **Calibration** and **System** tabs and are dependent on the type of base the ellipsometer is attached to and which attachments are installed. Some systems will not have a **Misc.** tab.

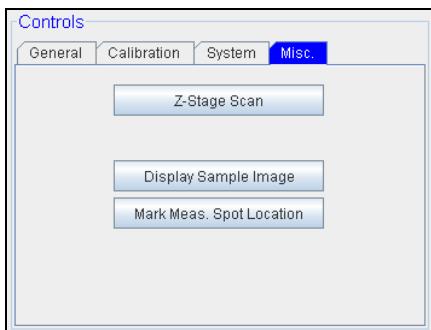


Figure 9-16. *Misc.* tab for ESM bases.

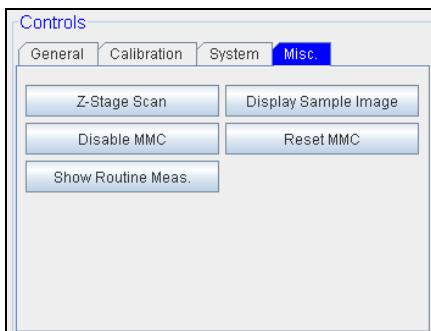


Figure 9-17. *Misc.* tab for AccuMap systems.

#### **Z-Stage Scan** (*Systems with motorized z-stages*)

This function scans the z-stage over a specified range and graphs the signal intensity versus z-stage position. This is especially useful when working with transparent substrates to determine if the backside beam is being collected.

#### **Display Sample Image** (*Systems with USB camera installed*)

Displays the camera image of the sample in a dialog. The dialog can stay open while other operations are performed.

#### **Mark Meas. Spot Location** (*Systems with USB camera installed*)

This function is used to mark the position of the ellipsometer probe beam on the camera image when the sample is aligned. After performing this function the "Show Beam" check box in the camera dialogs will provide an accurate representation of where the probe beam is intersecting the sample.

#### **Disable MMC** (*AccuMap*)

Pressing this button causes a user initiated fault on the translator. See the hardware manual for details on when this function may be used.

#### **Reset MMC** (*AccuMap*)

Pressing this button attempts to reset all translator faults. After pressing this button the translator is active and will move when commands are sent provided the door and all safety catches are engaged.

#### **Show Routine Meas.** (*AccuMap*)

Displays a dialog showing the results of routine measurements acquired on the Accumap. Routine measurements must be configured in the hardware configuration dialog.



# 10. Reference - Options Tab

The **Options** tab is shown in Figure 10-1. This tab consists of four panels: **Display Units**, **Configuration Controls**, **Miscellaneous**, and **About CompleteEASE**. A brief description of all commands within this tab is described.

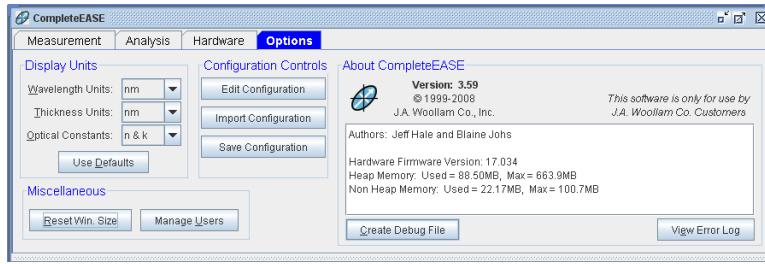


Figure 10-1. CompleteEASE software with the **Options** tab selected.

## 10.1. Display Units

Sets the “Wavelength Units.”, “Thickness Units”, “Optical Constants”, and “Graph Ellipsometric Data.” settings to their default values.

### Wavelength Units

Choose from Å, nm, µm, eV, and 1/cm for the wavelength units.

### Thickness Units

Choose from Å, nm, µm, and mm for the thickness units.

### Optical Constants

Display and report optical constants as either “n & k” or “e1 & e2”.

These settings are saved when the program is exited, and restored when the program is restarted.

## 'Use Defaults'

Return all settings to their default values, which include wavelength in nm, thickness in nm, and optical constants as "n & k".

## 10.2. Miscellaneous

### Reset Win. Size

Return the CompleteEASE window size to the default size.

### Manage Users

Press 'Manage Users' to setup the user list, along with access level and password, as shown in Figure 10-2. The user privileges can be defined for Engineer level, by further pressing 'Define User Privileges', which opens the window shown in Figure 10-3. The User customization is further defined in the CompleteEASE Configuration (next section).

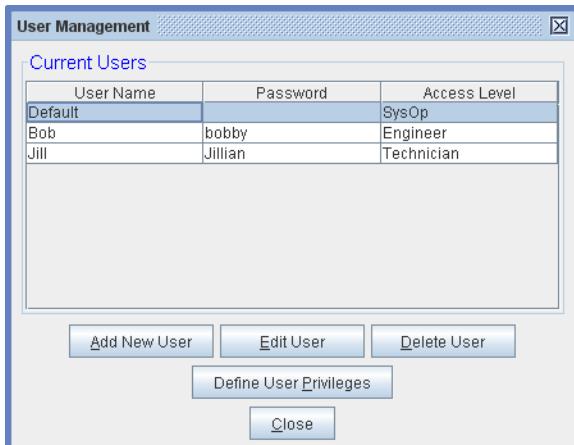


Figure 10-2. Manage Users window, where multiple users, passwords and privileges can be established.

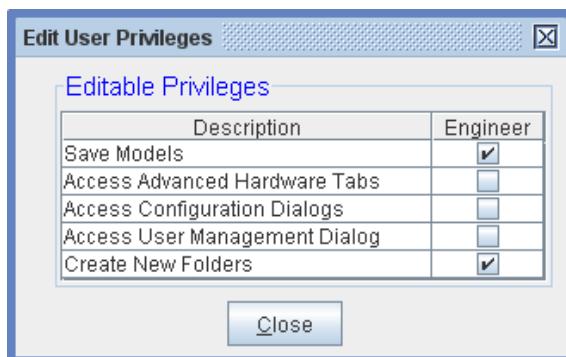


Figure 10-3. Define User Privileges for Engineer level.

---

## 10.3. Configuration Controls

### Edit Configuration

Allows customization of the CompleteEASE software configuration. Press this button to open the window shown in Figure 10-4. Each item to the left can be expanded by pressing the circle to the left of the name. Also, there are many hidden, Advanced options, which will not appear until you check the box at bottom of the screen: “Show Advanced Config. Options”. The list with Advanced options grows to that shown in Figure 10-5.

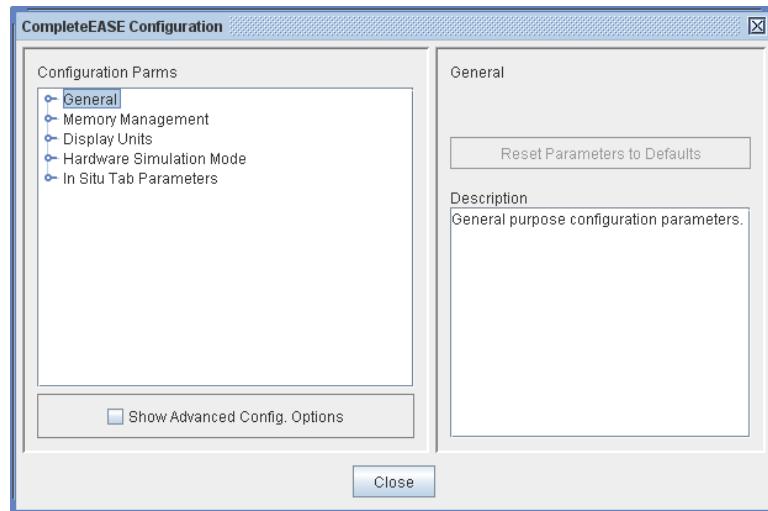


Figure 10-4. Edit Configuration window.

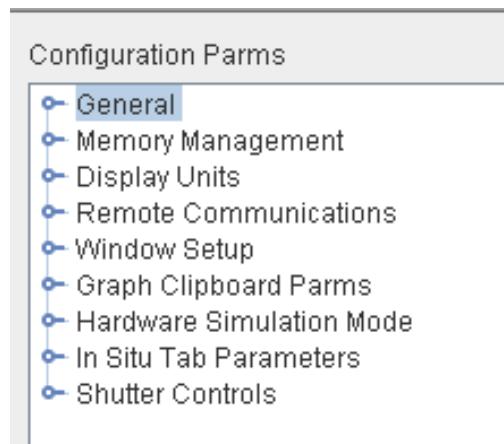


Figure 10-5. Edit Configuration window including Advanced Options.

Most of the settings within the CompleteEASE Configuration are self-explanatory and describe the default settings for the software. However, there are a few items of particular interest which will be discussed in this section.

## **General Configuration Parameters**

The general configuration parameters are shown in Figure 10-6. A description of each option appears when you press the individual line. User Log-In Mode and Users Have Own Folders are two options that are used when managing multiple users.

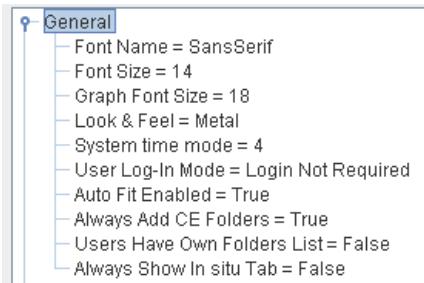


Figure 10-6. General Configuration Parameters.

## **Memory Management Configuration Parameters**

The memory is determined by the maximum number of wavelengths and maximum time slices allowed with in-situ data. See Figure 10-7.

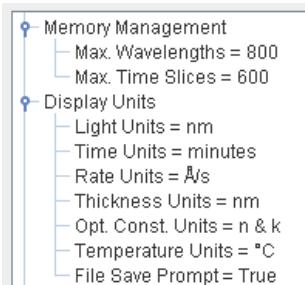


Figure 10-7. Memory Management and Display Units section of the Configuration Parameters window.

## **Display Units Configuration Parameters**

The Display Units section sets the default units for CompleteEASE. See Figure 10-7.

## **Remote Communications Configuration Parameters**

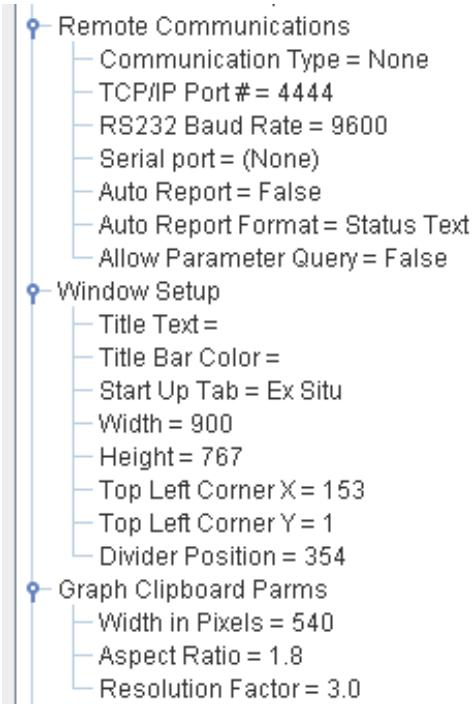
The Remote Communications section helps establish communication for CompleteEASE. See Figure 10-8.

## **Window Setup Configuration Parameters**

The Window Setup section sets the default window shape, size and location. See Figure 10-8.

## **Graph Clipboard Configuration Parameters**

The Graph Clipboard Params section sets the default graph dimensions and resolution when copying graphs to the clipboard. See Figure 10-8.



*Figure 10-8. Remote Communications, Window Setup, and Graph Clipboard Params sections of the Configuration Parameters window.*

### **Hardware Simulation Mode Configuration Parameters**

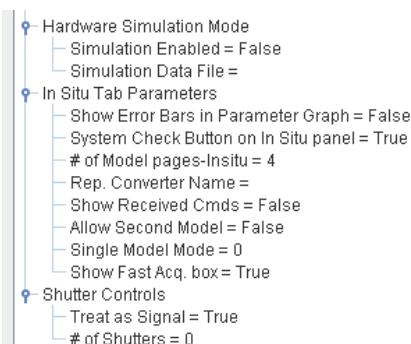
The Hardware Simulation Mode section sets whether hardware can be simulated when not attached. See Figure 10-9.

### **In Situ Tab Configuration Parameters**

The In Situ Tab Parameters section sets details regarding the In Situ Tab, which is generally hidden on systems that are not designated for in situ. See Figure 10-9.

### **Shutter Controls Configuration Parameters**

The Shutter Controls Parameters section sets details regarding in situ control of shutters for real-time process experiments. See Figure 10-9.



*Figure 10-9. Hardware Simulation Mode, In Situ Tab Parameters, and Shutter Controls sections of the Configuration Parameters window.*

## Import and Save Configuration

To copy the configuration from one computer to the next, you can ‘Save Configuration’ and then ‘Import Configuration’. This will help to setup the CompleteEASE software in the same way on multiple computers.

---

## 10.4. About CompleteEASE

Displays the “About” box shown in Figure 10-10, which contains the software version number, memory availability, and copyright information.

### Create Debug File

Click this button to create a debug file for sending in details to Woollam Company. The name is: *C:\CompleteEASE\CompleteEASE\_Debug.zip*. Email this file to your J.A. Woollam Co., Inc. representative to aid in debugging problems with your ellipsometer system.

### View Error Log

View the error log.



Figure 10-10. About Box.

# 11. Appendices

## 11.1. Troubleshooting Guide

Please contact your J.A. Woollam Co., Inc. representative with any questions relating to CompleteEASE or your ellipsometer system. To reduce the support time, please create and email the debug file described in the following section before contacting your representative.

Your closest Woollam Representative can be found in Section 11.3.

### Creating a Debug file

1. Click on the **Hardware** tab
2. Click on the “Error” button in the “Show Logs” section
3. Click on the “Save Debug File” button
4. The filename for the debug file is:  
*C:\CompleteEASE\CompleteEASE\_Debug.zip.*

Email this file to your J.A. Woollam Co., Inc. representative to aid in debugging problems with your ellipsometer system.

### Reporting Problems to the J. A. Woollam Co.

In the event that you have a problem with the EASE software or your hardware, we have made it very easy to gather information about your current setup to send to the Woollam Company. By following this procedure, your current configuration, log files, and recent calibration data will be zipped into a file called *CompleteEASE\_Debug.zip* that you can email to us along with a description of your problem and contact information. By providing all of this information in one place, we should be able to help you quickly identify the problem.

1. Choose ‘View Error Log’ from the ‘Help’ menu. This opens the log view.
2. Press the ‘Save Debug File’ button at the bottom of the dialog. This creates the file *CompleteEASE\_Debug.zip* in the \CompleteEASE directory.
3. Email the file along with a description of your problem and any supporting data to [support@jawoollam.com](mailto:support@jawoollam.com).

## 11.2. CompleteEASE Data Transfer (to/from WVASE32)

The data files in CompleteEASE™ and WVASE32™ are not directly compatible, as they have different file formats. The WVASE32 files are written in ASCII text, while the CompleteEASE files are “encrypted”. The file encryption in CompleteEASE is a “copy-protection” mechanism, as this software does not require an “activator key” to run, like WVASE32 requires.

If you have a copy of the WVASE32 software and the software key (activator) that accompanies it, you can easily import and export data files to modify their formats to be compatible with either WVASE32 or CompleteEASE.

The Experimental Data window is used to execute the data transfer of files already saved. Currently opened data is not modified.

Any data open in the Experimental Data window will be removed (deleted if not saved) by performing the following steps.

### Importing CompleteEASE Data to WVASE32:

1. From WVASE32, select “CompleteEASE Data Transfer” from the FILE menu of the EXPERIMENTAL DATA window and then select “Import Data from CompleteEASE”.

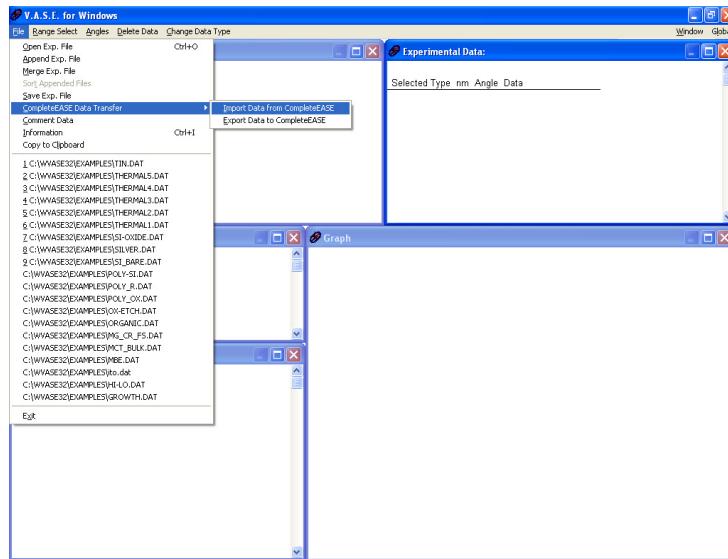


Figure 11-1. Choose the CompleteEASE Data Transfer menu from FILE menu of the Experimental Data Window.

2. Browse to select data files you wish to import from CompleteEASE. Multiple files can be selected.

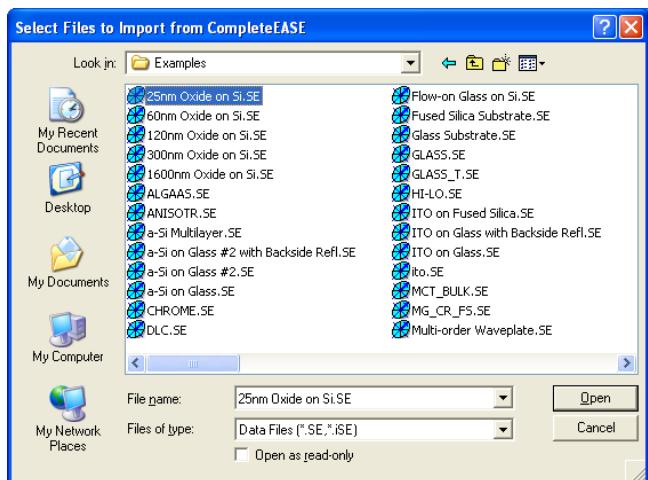


Figure 11-2. Select files you wish to Import.

3. Browse to select the directory where you wish the new files to be saved.  
Imported files will be saved in WVASE32 format in the directory chosen.

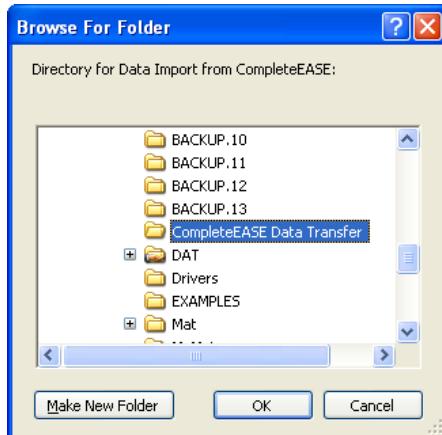


Figure 11-3. Choose the location to save imported data files.

4. After the files are imported, a message will appear, as in Figure 11-4.  
Previous ".SE" and ".iSE" files are now saved in WVASE32 ".dat" format.

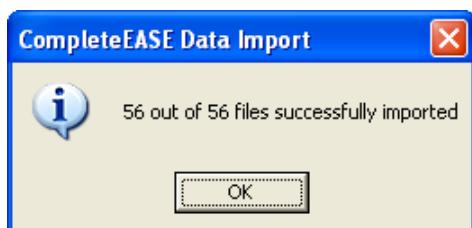


Figure 11-4. Message after all files imported correctly.

## Exporting WVASE32 Data to CompleteEASE:

1. From the Experimental Data window in WVASE32, select the file menu and choose “CompleteEASE Data Transfer”. Then, select the “Export Data to CompleteEASE” option as show in Figure 11-5.

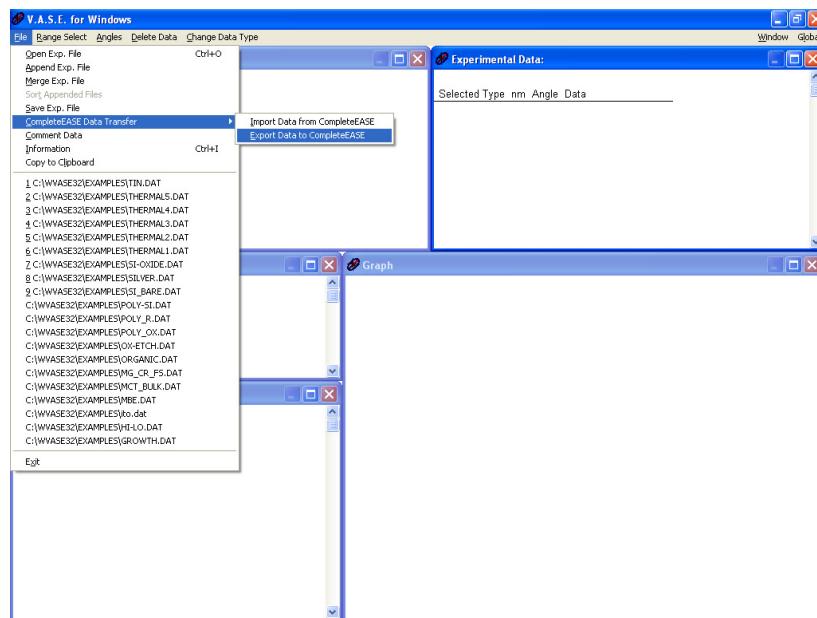


Figure 11-5. Selecting “Export Data to CompleteEASE”

2. Browse and select the WVASE32 data files for exporting to CompleteEASE, as in Figure 11-6. Multiple files can be selected.

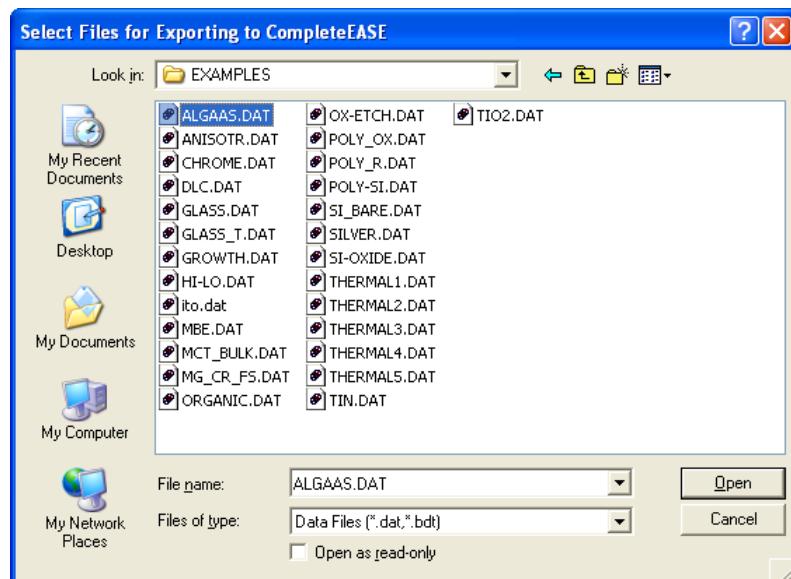


Figure 11-6. Choose WVASE32 data files you wish to export.

3. Browse to select the directory for data exported to CompleteEASE, as shown in Figure 11-7.. Exported files will be saved in CompleteEASE format in the directory chosen.

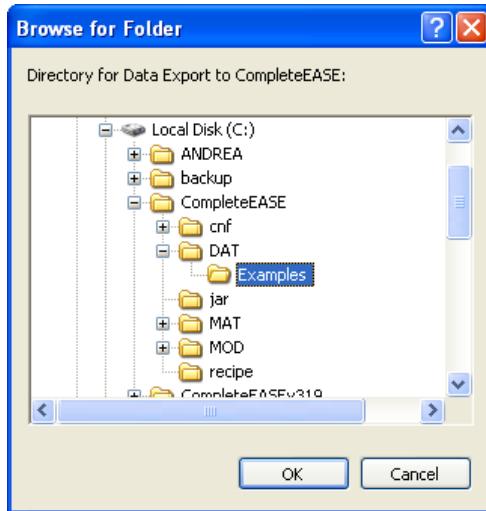


Figure 11-7. Browse for location to place the newly created CompleteEASE files.

4. After the files are exported, the following message will appear. Previous “.dat” and “.bdt” files are now saved in CompleteEASE “.SE” and “.iSE” formats.



Figure 11-8. Message when all data files are exported successfully.

---

## 11.3. Contacting the J.A. Woollam Co., Inc.

### J.A. Woollam Co., Inc.

645 M Street, Suite 102  
Lincoln, NE 68508 USA  
PHONE: 402-477-7501  
FAX: 402-477-8214  
Sales@jawoollam.com or Support@jawoollam.com  
www.jawoollam.com

---

#### Germany & Europe

L.O.T.-Oriel GmbH  
Im Tiefen See 58  
Darmstadt 64293 Germany  
PH: 49-6151-880668  
FX: 49-6151-896667  
wagner@lot-oriel.de  
www.lot-oriel.com

#### United Kingdom

L.O.T.-Oriel UK & Ireland  
1 Mole Business Park  
Leatherhead, Surrey  
United Kingdom KT227 BA  
PH: 44-1372-378822  
FX: 44-1372-375353  
heath@lotoriel.co.uk  
www.lotoriel.co.uk

#### France

L.O.T. Oriel France  
4, Allée des Garays  
Palaiseau, France 91120  
PH: 33-1-69194949  
FX: 33-1-69194930  
serre@lot-oriel.fr  
www.lot-oriel.fr

#### Italy

L.O.T. Oriel Italy  
Via Francesco Saporì 27  
Rome, Italy 00143  
PH: 39-06-5004204  
FX: 39-06-5010389  
schutzmann@lot-oriel.it  
www.lot-oriel.it

#### Japan

J.A. Woollam Japan  
Fuji 2F 5-22-9 Ogikubo  
Suginami-ku  
Tokyo 167-0051 Japan  
PH: 81-3-3220-5871  
FX: 81-3-3220-5876  
info@jawjapan.com  
www.jawjapan.com

#### Korea

Wizoptics  
#501, Taebo B/D  
240-5 Gocheon-Dong  
Uiwang-si, Gyeonggi-do  
437-801 Korea  
PH: 82-31-477-3785  
FX: 82-31-477-3786  
info@wizoptics.com  
www.wizoptics.com

#### Singapore

Crest Technology  
4 Loyang Street  
Loyang Industrial Estate  
508839 Singapore  
PH: 65-6546-4811  
FX: 65-6546-4822  
marcus@crest-technology.com  
www.crest-technology.com

#### India

Sinsil International  
New Bramhand Annex  
Phase 8, G7/G2  
Thane (W) 400607  
Mumbai, India  
PH: 91-22-2489-5077  
FX: 91-90-2722-5513

#### China

Lamda Pacific  
Room 906, Block C  
No. 70 CaoBao Rd.  
Shanghai, 200235, China  
PH: 86-21-64325169  
FX: 86-21-64326125  
sales@lamdapacific.com  
www.lamdapacific.com

#### Taiwan

Titan Electro-Optics Co.  
14 Fl., No. 19-11  
San-Chung Road  
Taipei 115, Taiwan  
PH: 886-2-2655-2200  
FX: 886-2-2655-2233  
sales@teo.com.tw  
www.teo.com.tw

#### Australia

Scientific Solutions  
P.O. Box 4033  
Caloundra BC  
Queensland, Australia 4551  
PH: 61-7-5438-2222  
FX: 61-7-5438-2233  
info@scisol.com.au  
www.scisol.com.au

#### Israel

VST Service Ltd.  
P.O. Box 4137  
19 Imber Street  
Petach-Tikva, 49130 Israel  
PH: 972-3-92477-10  
FX: 972-3-92477-11  
angel@vacuumltd.com  
www.vacuumltd.com

---

## A

Absorbing Thin Films · 93, 104, 113  
Add · 207  
Adding New Folders · 14, 17  
Alloy Files · 181  
Ambient Index > 1 · 233  
Analysis Tab · 203  
Angle Offset · 211  
Append Data · 69

---

## B

Backside reflections · 75  
Backside Reflections · 68  
Bandwidth (nm) · 147  
B-SPLINE · 107, 223

---

## C

Calibration · 244  
Cauchy · 63, 142, 216  
Cauchy\_WVL · 217, 218  
Changing the Graph · 155  
Clear Multi-Data Set Mode · 158  
Cody-Lorentz · 124, 231  
Compare Optical Constants · 89  
Comparing Results · 88  
Composition Library · 228  
Configuration Controls · 255  
Configure Options · 241  
Create Debug File · 258

---

## D

**Data Analysis** · 44, 46  
Data Transfer (to/from WVASE32) · 260  
Debug file · 259  
Delete · 207  
Delta Offset · 233  
Depolarization · 73, 75  
Derived Parameters · 57, 236  
Display Units · 253  
Drude · 231

---

## E

Editing Layers · 208  
Effective Medium Approximation · 48, 215  
Ellipsometry · 22  
EMA · *See* Effective Medium Approximation  
Error Logs · 244  
Exporting WVASE32 Data · 262

---

---

## F

File Structure · 13  
Fit · 204  
Fit Dynamic · 205  
Fit Log · 87  
FIT Options · 234  
Fit Results · 55  
Fit Scan Data · 144  
Fit Weight · 236  
Fitting the Data · 50

---

## G

Gaussian · 230  
Generalized SE · 192  
Generate · 204  
Generate Report · 90  
Gen-Osc · 114, 221, 230  
Glass with Absorbing Film · 122  
Glass with Transparent Film · 79  
Global Fits · 66, 111, 235  
Graded Layer · 49, 81, 220  
Graph · 193  
Graph All Data Sets · 155  
Graph ScratchPad · 70, 135, 196

---

## H

Hardware Tab · 242  
Harmonic · 230  
HTML Clipboard · 87

---

## I

Importing CompleteEASE Data · 260  
Include Depolarization Data · 148, 236  
Include Intensity Data · 236  
Include Substrate Backside Correction · 232  
Include Surface Roughness · 208  
Installing the Software · 7  
Intermix · 228

---

## L

Limit Wvl Range for Fit · 111  
Lorentz · 230

---

## M

Manage Users · 254

---

**Map Data** · 137, 139  
Measurement Tab · 198  
Metal Substrates · 95  
Mode: · 198  
Model · 47  
Model Calculation · 145, 232  
MODEL Options · 232  
MSE · 49  
Mueller-Matrix · 192  
Multi-Layer (empty) Model · 151  
**Multiple Data Types** · 94, 132  
Multi-Sample Analysis · 150, 157, 162, 233

---

## N

N, C, & S · 50

---

## O

Off-Sample Baseline · 244  
Options Tab · 253  
OTHER Options · 239

---

## P

Parameter Error Bars · 55  
**Parameter Uniqueness** · 101, 132, 240  
Parameterize · 113  
Park Z-Stage · 242  
Perform Thickness Pre-Fit · 235  
Pole · 230  
Pseudo Optical Constants · 47

---

## R

Range-Select · 194  
Range-Selecting Wavelengths · 109  
Re-analyzing Multiple Data Sets · 90  
Re-initialize · 242  
Return Path Ellipsometer · 233  
Roughness · 131

---

## S

Sample Alignment: · 199  
**Save** · 98, 208  
Saving a Model · 127  
Screen Layout · 193  
SE + T · 94, 132  
Selecting a Point · 140  
Selecting Multiple Points on a Map · 154  
Self-Assembled Monolayers · 100  
Sellmeier · 143, 218  
Set Ranges · 142

---

Set Symbol Size · 152  
SETUP Program · 7  
Short-cut · 21  
Show Data · 194  
Show Symbols · 197  
Si Model · 57  
Si with Absorbing Film · 105  
Si with Transparent Film · 64  
Signal · 243  
**Simulate Data** · 241  
Source and Receive Rot. · 233  
S-T Baseline · 244  
Starting Mat · 123  
Statistics · 195  
Surface Roughness · 81  
System Status · 198

---

## T

Tabulated n,k · 215  
Tauc-Lorentz · 231  
Thickness Non-Uniformity · 146  
Thickness Pre-fitting · 59  
Transmission Data % Weight · 236  
**Transparent Films** · 45, 79  
Transparent Substrates · 68  
**Transparent Thin Films** · 44, 63  
Troubleshooting · 259  
**Try Alternate Models** · 83, 239

---

## U

Uniaxial · 229  
Uniaxial-Diff · 229  
Use Clipboard Aspect Ratio · 197

---

## V

View Previous Fit Results · 201  
Visualizing Model Changes · 62

---

## W

Wavelength Range Expansion · 109  
Wavelength Units – eV · 140  
Wvl Shift (nm) · 233  
**Wvl. Range Expansion Fit** · 239

---

## Z

Zoom All · 194  
Zooming on Map · 153  
Z-Stage Scan · 243

---