# Manual for the XPD Package

## Content

The XPD package, powered by the IGOR Pro, is designed to acquire, analyze, and process XPD data. It is designed to be user-friendly. Its graphical interface let users do all operations just by mouse clicking.

**1. Installation or update of the XPD package**

Installation of the XPD package is quite easy. Just make sure the IGOR Pro is not running and copy the package's IGOR procedure file "XPD.ipf" to the current user's "IGOR Procedures" folder. For example, if the current user name is XPS, then copy the file "XPD.ipf" to directory: C:\Users\XPS\Documents\WaveMetrics\IGOR Pro 6 User Files\IGOR Procedures.

If the package's codes have been changed and the package has to be updated, just copy the latest "XPD.ipf" to the current user's "IGOR Procedures" folder and overwrite the old "XPD.ipf".

For temporary test, open "XPD.ipf" with a text editor, copy the text of "XPD.ipf" and paste it into the IGOR Pro's Procedure Window (use Ctrl + M shortcut key to create a new Procedure Window), click the "Compile" button at the bottom of the Procedure Window to compile the procedure, then the XPD package is ready to be tested.

**2. Starting the XPD package**

Start the IGOR Pro program and the IGOR Pro will automatically load and compile the XPD package if the XPD package has been installed. An "XPD" menu is added to the menu bar of the IGOR Pro as shown in a screenshot of the IGOR Pro just after starting (Fig. 1).

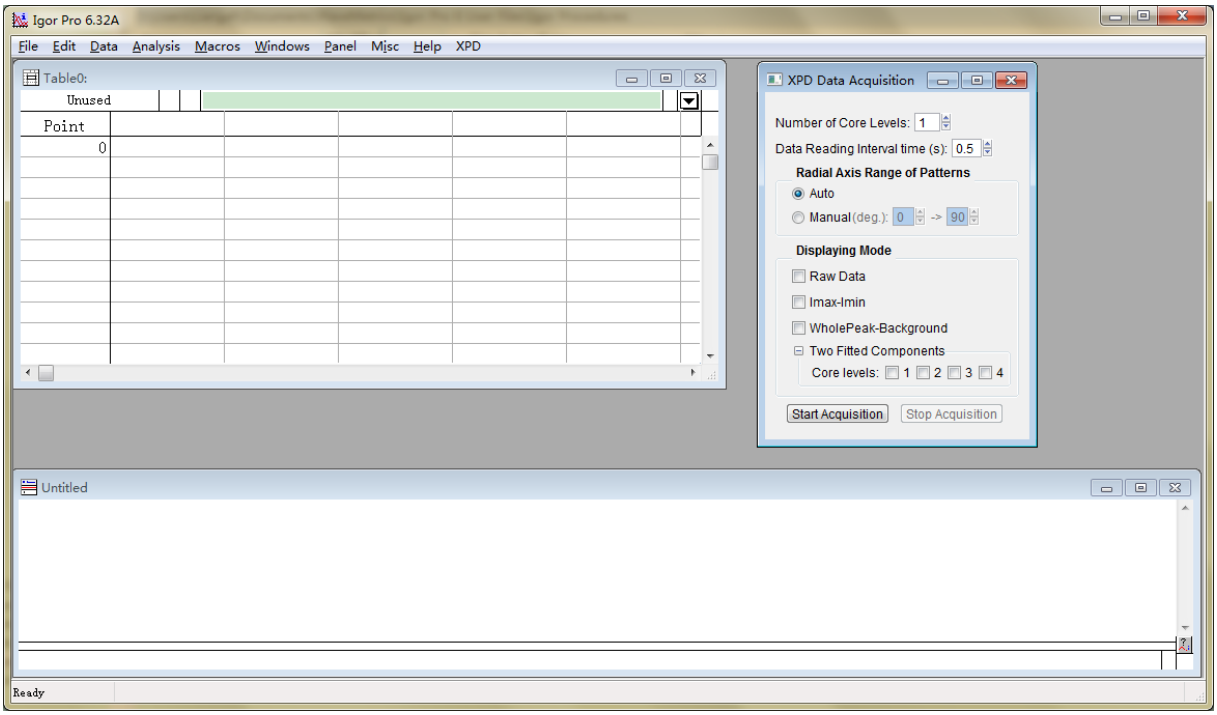


Fig. 1. The screenshot of the IGOR Pro with the installed XPD packaged. The “XPD” menu is on the menu bar of the IGOR Pro.

Click the “XPD” menu and the main entry into the tools provided by the XPD package is shown in the submenu (Fig. 2).

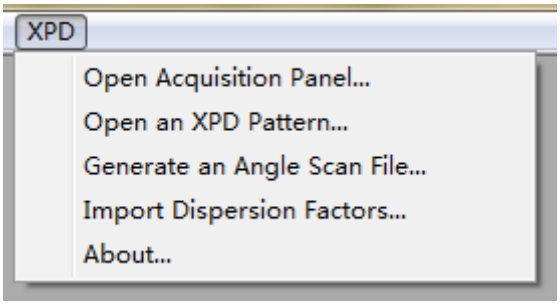


Fig. 2. The “XPD” menu.

Clicking on the ‘Open Acquisition Panel…’ submenu will open the ‘XPD Data Acquisition’ panel (Fig. 3) for data acquisition and XPD pattern displaying. For convenience, an acquisition panel is automatically loaded and displayed at the startup (Fig. 1).

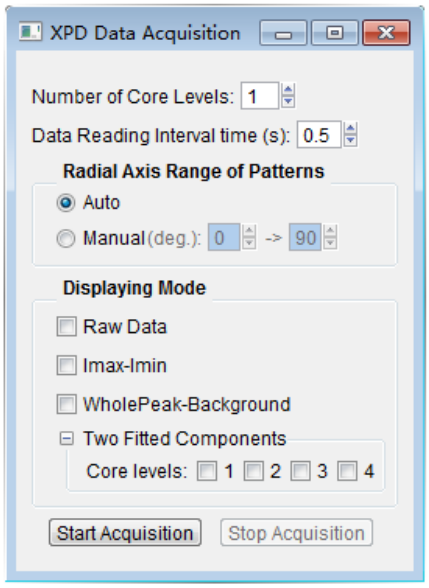


Fig. 3. The acquisition panel.

Clicking on the 'Open an XPD Pattern…' submenu will bring up a file open dialog to let users open a data file (*.xpd) that contains the data of an XPD pattern for processing and analyzing.

Clicking on the 'Generate an Angle Scan File…' submenu will open the 'Generate Angle Scan Files' panel for generating series of variable step size scan angles, see Section 7.

The 'Import Dispersion Factors…' submenu is used to import the dispersion factors of the Omicron Argus analyzer's detector. Detailed information about importing dispersion factors is described in Section 8.

| Note |
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| Help message for each button of a panel is displayed on the status bar of the IGOR Pro window when the cursor is on the button. |

**3. Data acquisition**

Users can define the data acquisition parameters via the 'XPD Data Acquisition' panel (Fig. 3).

The 'Number of Core Levels' is the number of the core levels that will be measured at every angular position. Up to 12 core levels are supported. For example, if O 1*s*, Ti 2*p*3/2, Ba 4*d* will be measured at each angular position, then the 'Number of Core Levels' is 3.

The ‘Data Reading Interval time’ is how often the IGOR Pro will read the data file saved by the MATE script of the MATRIX. Minimum interval time is 0.5 seconds, maximum interval time is 60 seconds.

The ‘Radial Axis Range of patterns’ is the Polar angular range of all XPD patterns when displaying XPD patterns.

The ‘Displaying Mode’ is what data will be displayed on an XPD pattern, which determines how to calculate the data point intensity of an XPD pattern. Four modes are supported:

(1) ‘Raw Data’ mode: the area of the core level peaks will be used as the data point intensity of an XPD pattern without fitting or background subtraction. For example, the gray color depicts the area of a core level peak in Fig. 4.

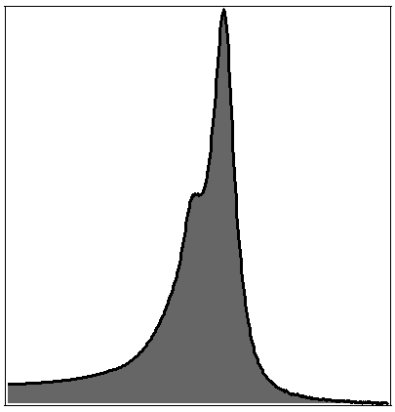

Fig. 4. ‘Raw Data’ mode.

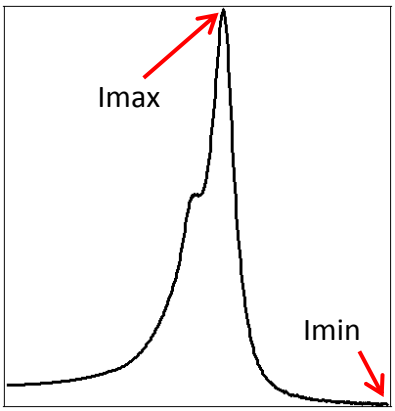


Fig. 5. ‘Imax-Imin’ mode.

(2) ‘Imax-Imin’ mode: the difference of the maximum intensity and the minimum intensity of the core level peaks will be used as the data point intensity of an XPD pattern. For example, in Fig. 5, the intensity at the top of the peak is Imax, the intensity at the right hand side is Imin.

(3) ‘WholePeak-Background’ mode: firstly the background of a core level peak is subtracted by Shirley algorithm, and then the area of the core level peak without background is used as photoelectron intensity. The gray color is the area in Fig. 6.

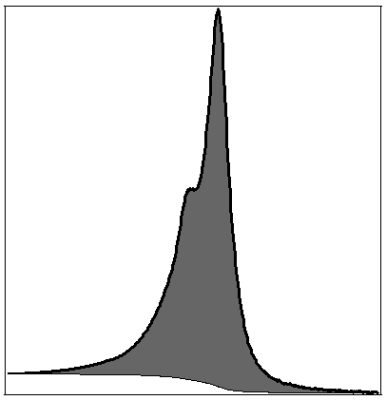

Fig. 6. ‘WholePeak-Bkg’ mode.

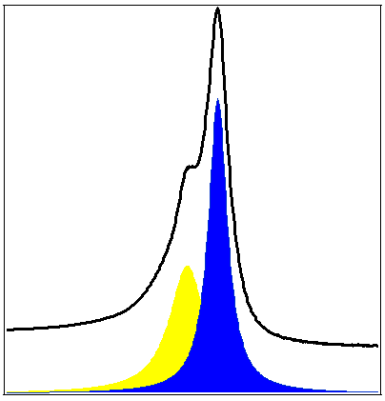

Fig. 7. ‘Two Fitted Components’ mode.

The above three modes are applied to all core levels.

(4) ‘Two Fitted Components’ mode: firstly the background of the core level peaks is subtracted by Shirley algorithm, and then the core level peaks without background is fit by using 2 Voigt line shapes, finally the area of the two fit line shapes are used as photoelectron intensities and displayed separately on two patterns. In Fig. 7, the yellow fitted peak at left hand side is Left Component (its right hand side is covered by the blue fitted peak), and the blue fitted peak at right hand side is Right Component.

Up to four core levels (the first four core levels) are supported for ‘Two Fitted Components’ mode. Just click the corresponding sequence number of the core levels to select the ‘Two Fitted Components’ mode.

Click the "Start Acquisition" button to start the acquisition. If it’s the first time to start acquisition after the XPD package installation, an open dialogue will pop up to ask the user to import dispersion factors, otherwise, an open dialogue will pop up to let user select the data file (*.csv) that contains the XPD data.

If there are no data in the file, a message "No data in the file, waiting for data acquisition..." is displayed in the history area of the command window of the IGOR Pro.

If there are data in the file, the package will read and process the data (core level name (transition name in the CASCADE), center energy, pass energy, theta angle, phi angle and the counts of each channel) and display XPS spectra and XPD patterns (Fig. 8). The color scale of XPD patterns will be shown under the Acquisition panel window (Fig. 9).

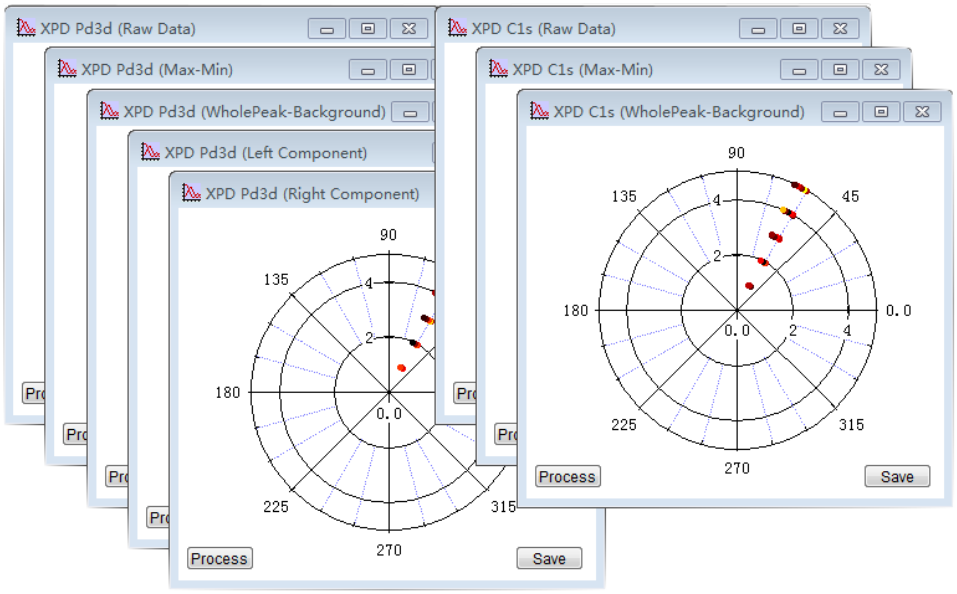


Fig. 8. XPD patterns.

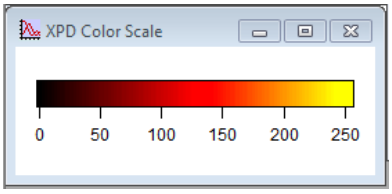


Fig. 9. The color scale of XPD patterns.

If the 'Two Fitted Components' displaying mode of a core level has been selected, the package will wait for users to specify the position of two peaks for fitting when displaying the core level's XPS spectrum at the first time as shown in Fig. 10. Once users specify two peaks, the package will automatically do the fitting automatically for all the spectra of the selected core levels as shown in Fig. 11.

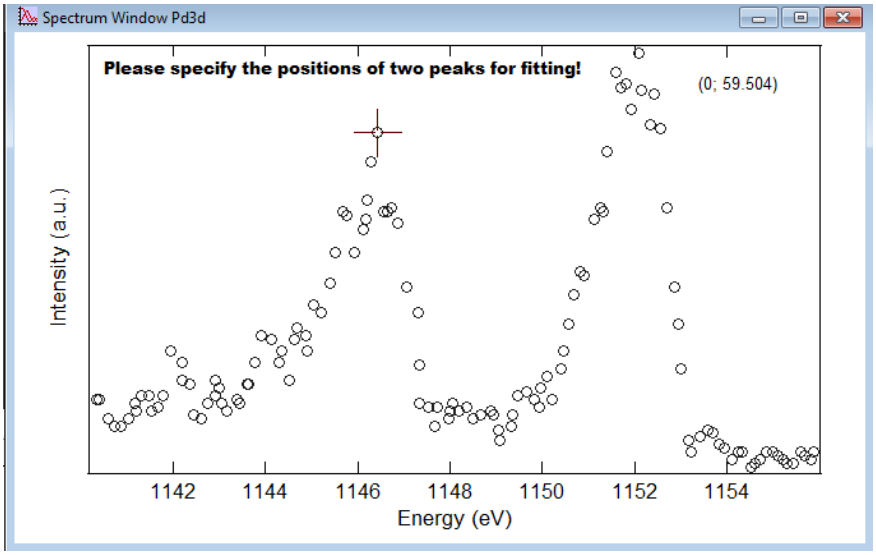


Fig. 10. The package is waiting for users to specify the position of two peaks for fitting.

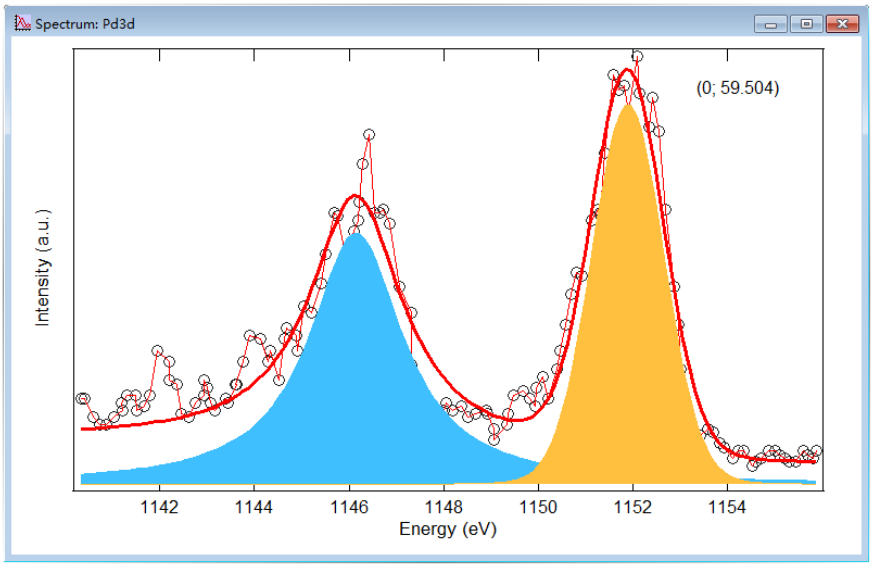


Fig. 11. The core level spectrum (after background subtraction) has been fitted by two Voigt line shapes.

The number of the spectra is displaying in the history area of the IGOR's command line window.

When an XPD experiment is done, stop the acquisition by clicking "Stop Acquisition". Save the IGOR experiment and all the data will be saved in an IGOR's experiment file.

Click the "Save" button at the bottom-right corner of a pattern windows (Fig. 8), the data of the XPD pattern can be saved separately into a text file (*.xpd).

| Note |
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| The package is able to automatically count the number of the core levels in the data file. If it finds that the number of core levels in the data file is NOT equal the input values (the 'Number of Core Levels' in the data acquisition panel), the package will prompt a message box (Fig. N-1) and abort. The number of core levels in the data file will be displayed in the command window. |

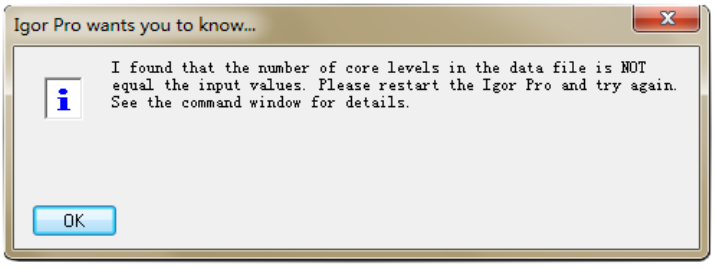


Fig. N-1. Message box: the number of core levels in the data file is not equal the input values.

**4. Processing of XPD patterns**

Click the "Process" button at the bottom-left corner of an XPD pattern window (Fig. 8), the pattern will be displayed in a new window and the Process & Analysis Panel will display next to the pattern window at the same time as shown in Fig. 12.

When a data point of the XPD pattern is clicked, the data point's theta angle, phi angle, and intensity will be shown at the bottom of Process & Analysis panel.

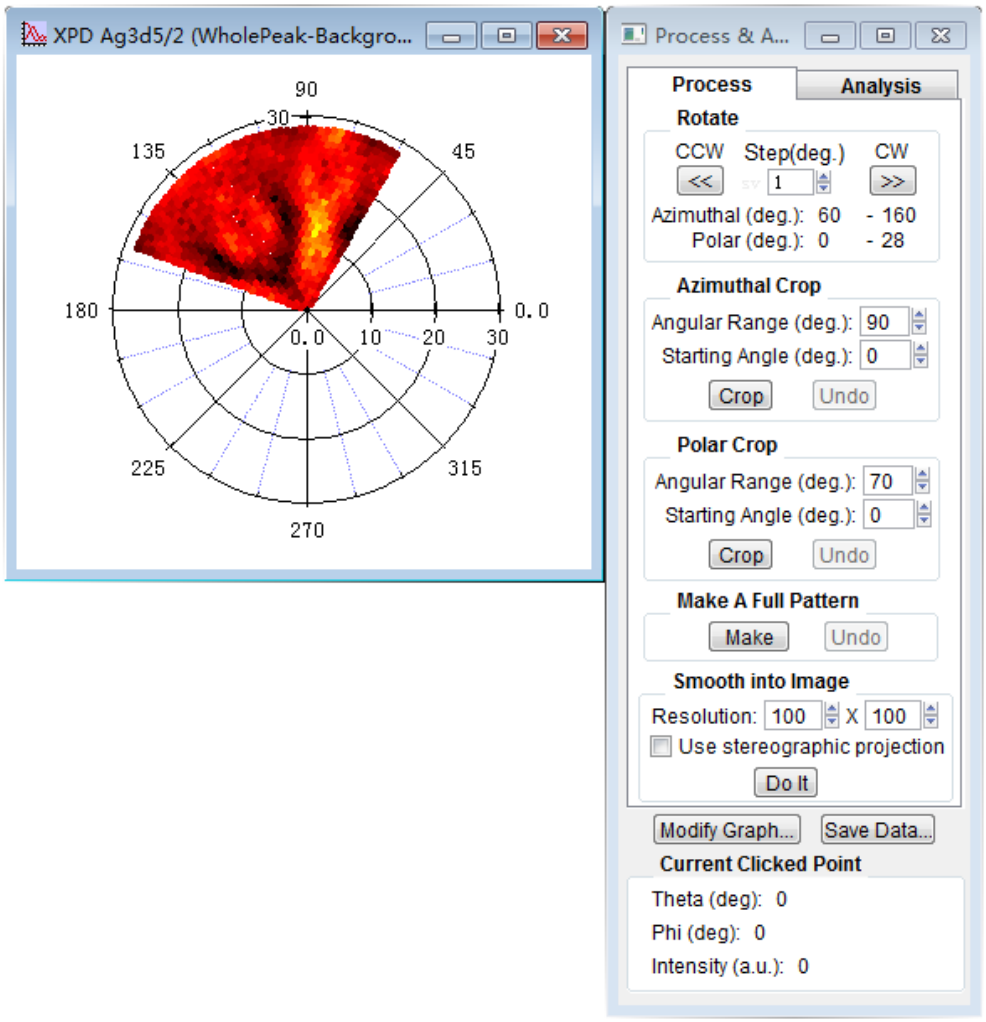


Fig. 12. The Process tab and an XPD pattern. The tiny white dots in the pattern are space between data points.

| Note |
| --- |
| In this manual, theta angle is polar angle, and phi angle is azimuthal angle. |

| Note |
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| When a data point of the XPD pattern is clicked, the data point's phi angle and theta angle are also shown in corresponding input boxes, e.g., the "Starting Angle (deg.)" input boxes of the "Azimuthal Crop" group boxes. So users can input angles just by clicking a data point of the XPD pattern. |

### 4.1. Rotate a pattern

Click the "<<" or ">>" button in the "Rotate" group box, the XPD pattern will rotate counter clock-wise or clock-wise respectively, and the corresponding azimuthal and polar angular range will update at the same time in the "Rotate" group box. The pattern in Fig. 13 has been rotated 8 deg. counter clock-wise with respect to the pattern in Fig. 12.

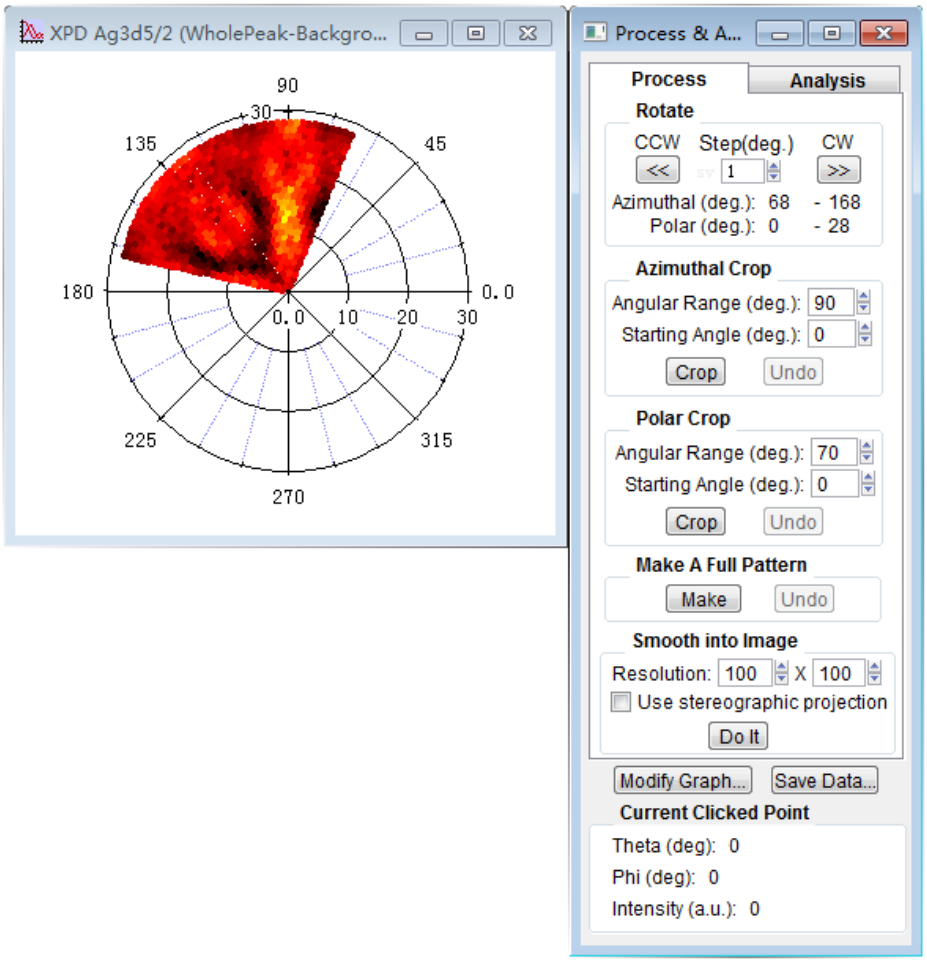


Fig. 13. The Process & Analysis Panel and a rotated XPD pattern. The pattern has been rotated 8 deg. counter clock-wise with respect to the pattern in Fig. 12.

### 4.2. Azimuthal crop

In the “Azimuthal Crop” group box, click the “Crop” button to azimuthally crop the XPD pattern to a pattern of the “Angular Range” from the “Starting Angle”, which means the data points outside the “Angular Range” will be deleted. The pattern in Fig. 14 has been cropped to the azimuthal range of 90 degrees.

Click the “Undo” button to undo the crop.

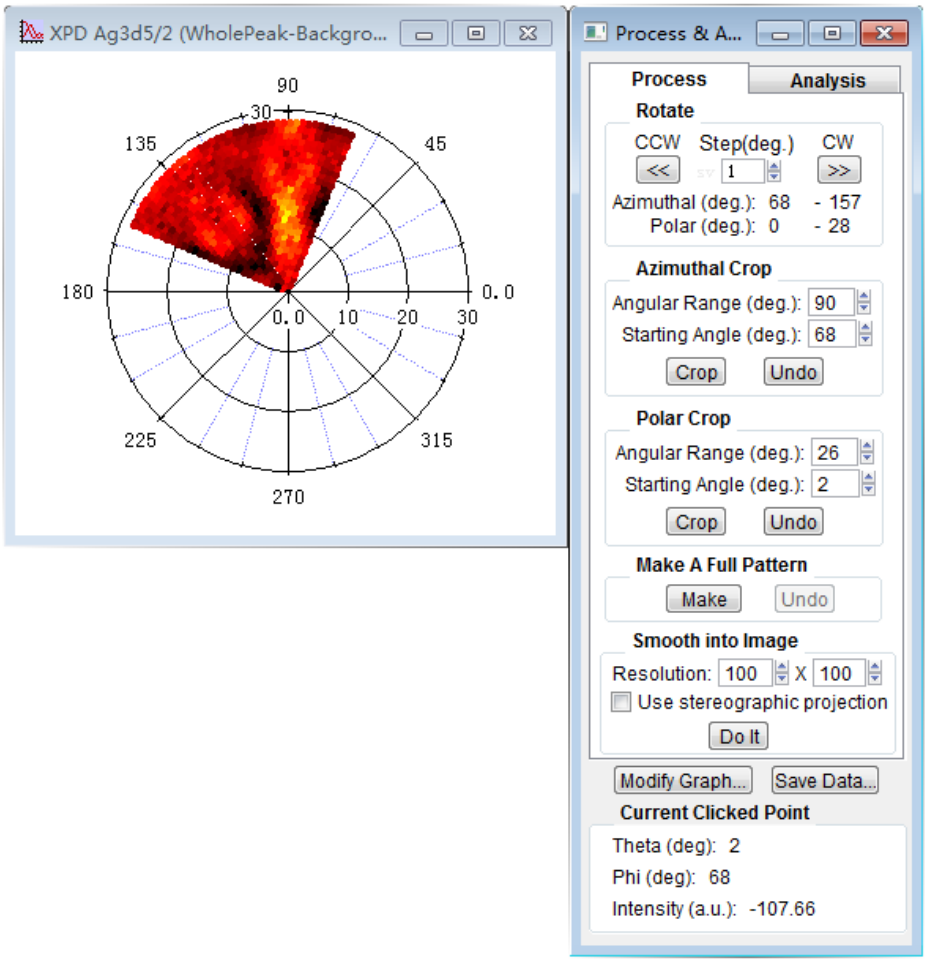


Fig. 14. A pattern cropped to the azimuthal range of 90 degrees.

### 4.3. Radial crop

In the “Radial Crop” group box, click the “Crop” button to radially crop the XPD pattern to a pattern of the “Angular Range” from the “Starting Angle”, which means the data points outside the “Angular Range” will be deleted. The pattern in Fig. 15 has been cropped to the polar range of 26 degrees.

Click the “Undo” button to undo the crop.

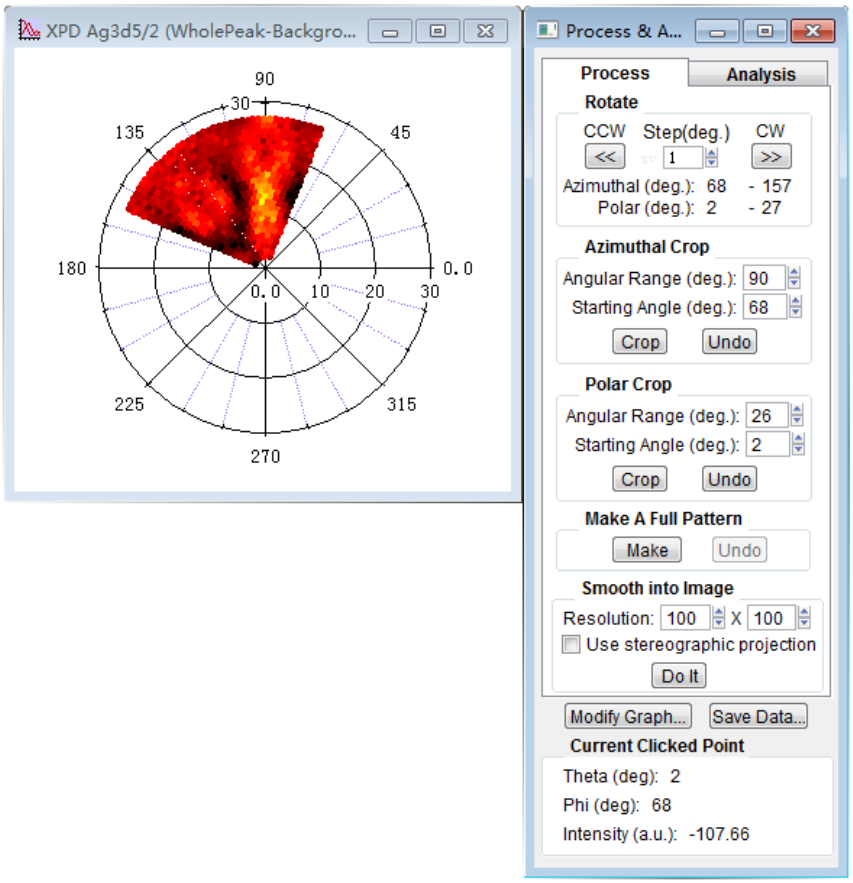


Fig. 15. A pattern cropped to the radial range of 26 degrees.

### 4.4. Make a full 2π pattern

Click the "Make" button in the “Make A Full Pattern” group box, the pattern will be duplicated and rotated counter clock-wise to form a new pattern of full 2π as shown in Fig. 16.

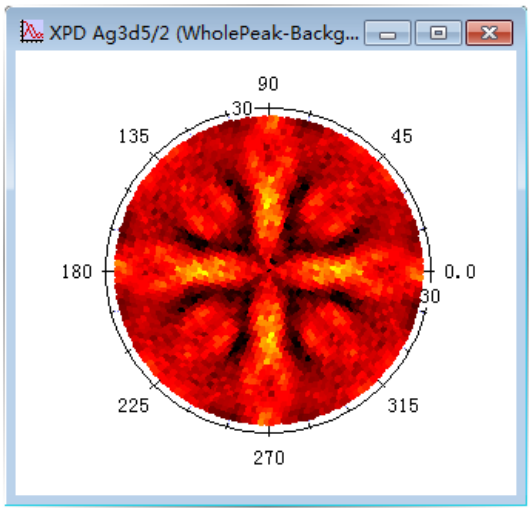


Fig. 16. A full 2π pattern.

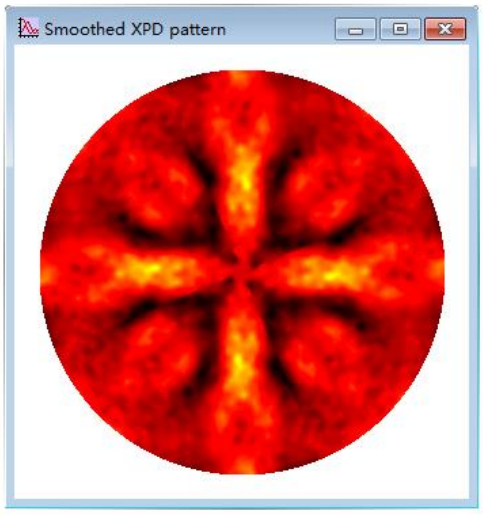


Fig. 17. A smoothed image of an XPD pattern.

### 4.5. Interpolate and smooth a pattern and convert it to an image for publication

Input the resolution in the “Smooth into Image” group box, and click the “Do It” button, the XPD pattern will be interpolated, smoothed, and converted to an image for publication. Up to 1000 x 1000 pixels of resolution are supported. The resolution of the image in Fig. 17 is 300 X 300.

If users hope to make a pattern image by using stereographic projection method, select the “Use stereographic projection” before click “Do It” button. The pattern will be transformed to a pattern used stereographic projection firstly (the pattern in the window beside the Process & Analysis panel will be contracted to a dot), and then converted to an image.

| Note |
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| The higher the resolution is, the more time it takes to process the interpolation. For example, it may take a few minutes if the resolution is 600 X 600. |

The data of interpolated image is stored in a 2D matrix named ‘SmthImgEqPrj’ (for azimuthal equidistance polar projection) or ‘SmthImgStgPrj’ (for azimuthal equidistance polar projection). The 2D matrix is placed in the folder root:Packages:XPD:Process. Advanced users are able to further process the image by employing the IGOR Pro’s built-in powerful tools (e.g. ‘MatrixFilter’ operation) or other software.

## 5. Analysis of XPD patterns

Click the “Analysis” tab next to the “Process” tab (Fig. 12) in the Process & Analysis panel, the Process tab will change to Analysis Tab as shown in Fig. 18. The “Polar Angle” and “Azimuthal Angle” input boxes in the Analysis tab show the theta angle and phi angle of the current clicked data point respectively.

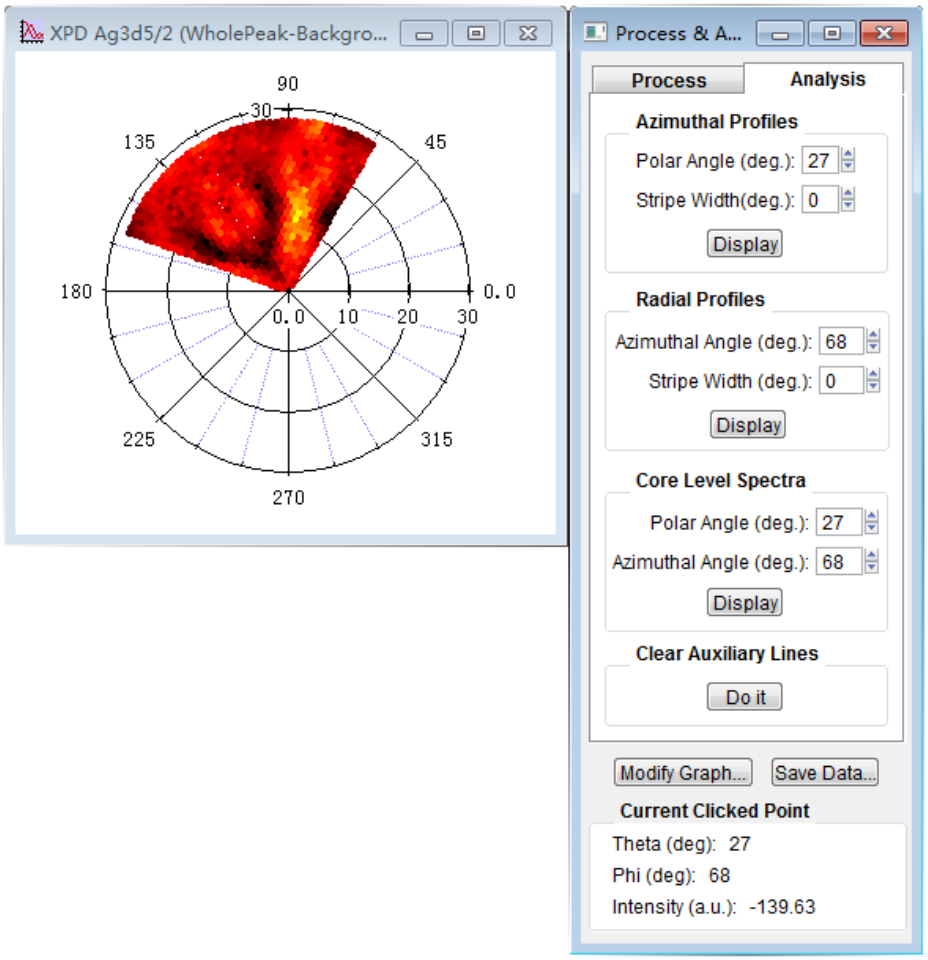



Fig. 18. The Analysis tab and an XPD pattern.

| Note |
| --- |
| When a data point of the XPD pattern is clicked, the data point's theta angle and phi angle are also shown in the "Polar Angle (deg.)" and "Azimuthal Angle (deg.)" input boxes of the Analysis tab respectively. So users can input the polar or azimuthal angles just by clicking a data point of the XPD pattern. |

### 5.1. Display azimuthal profiles

Input the polar angle along which the azimuthal profile will display, or click a data point of the pattern, the data point's polar angle will show in the "Polar Angle (deg.)" input box (Fig. 18).

Click the "Display" button in the "Azimuthal Profiles" box, a blue circle (if Stripe Width = 0, Fig. 19) whose polar angle is equal the input polar angle or two blue circles (if Stripe Width > 0, Fig. 20) whose centerline's polar angle is equal the input polar angle will display

on the pattern and the corresponding profile curve will display in a graph window at the same time (Fig. 19, Fig.20). The Stipe Width is the polar angle difference of the two circles. If Stipe Width = 0, the profile points are the data points or the interpolated data points along the blue circle. If Stripe Width > 0, the value of each profile point is the average value of the data points or the interpolated data points that have the same phi angle among the stripe.

Click the up or down arrows of the “Polar Angle (deg.)” or the “Stipe Width (deg.)” input box, the values in the input box, the blue circles, and the profile curve will change simultaneously.

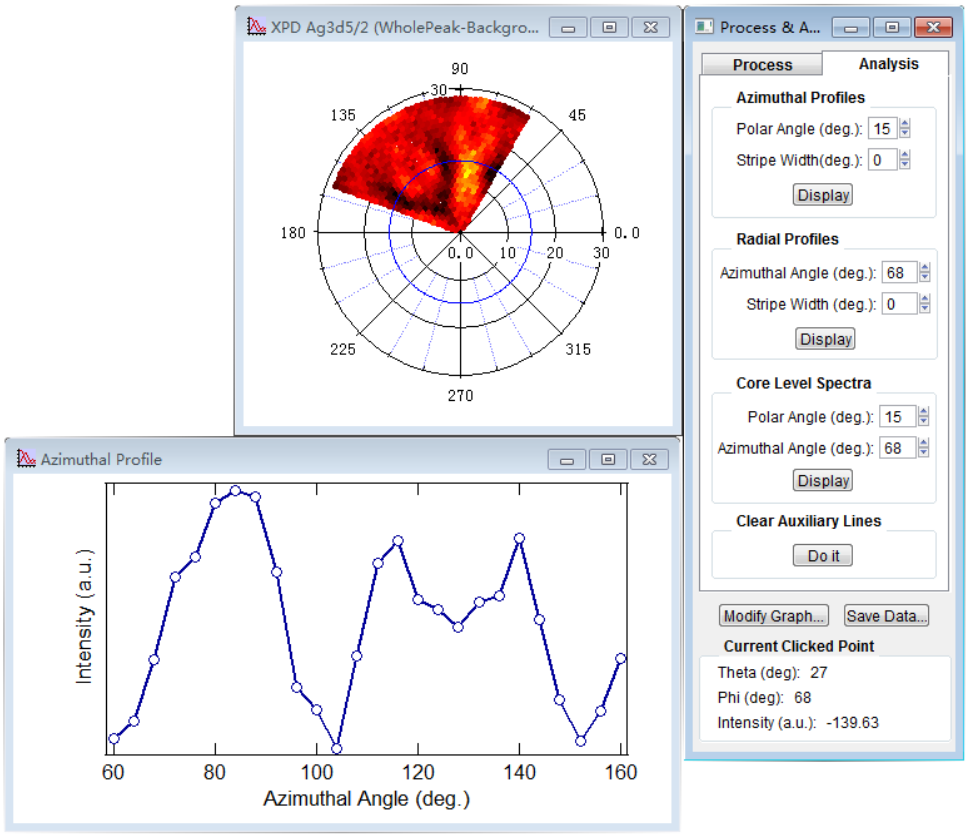



Fig. 20. A blue circle shown on the pattern (Stripe Width = 0) and the corresponding azimuthal profile curve displays in a graph window.

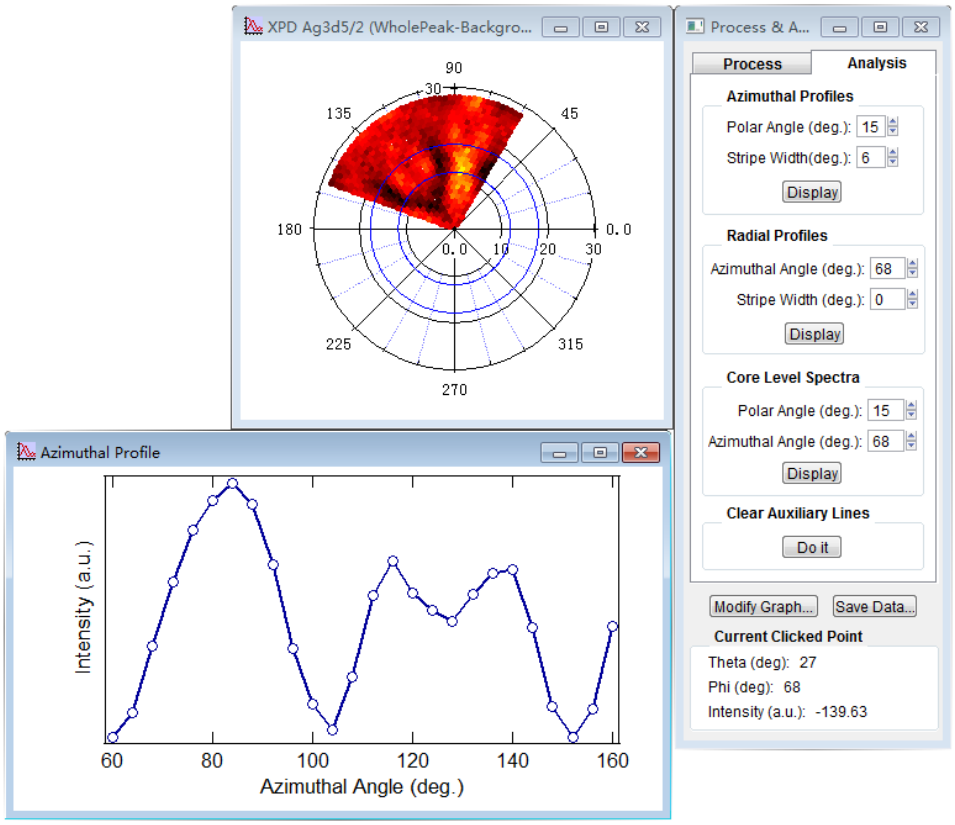



Fig. 21. Two blue circles shown on the pattern (Stripe Width > 0) and the corresponding azimuthal profile curve displays in a graph window.

### 5.2. Display radial profiles

Input the azimuthal angle along which the radial profile will display, or click a data point of the pattern, the data point's azimuthal angle will show in the "Azimuthal Angle (deg.)" input box (Fig. 18).

Click the "Display" button in the "Radial Profiles" box, a blue line (if Stripe Width = 0, Fig. 21) whose azimuthal angle is equal the input azimuthal angle or two blue lines (if Stripe Width > 0, Fig. 22) whose centerline's azimuthal angle is equal the input azimuthal angle will display on the pattern and the corresponding profile curve will display in a graph window at the same time (Fig. 21, Fig.22). The Sector Width is the included angle of the two lines. If Sector Width = 0, the profile points are the data points or the interpolated data points along the blue line. If Stripe Width > 0, the value of each profile point is the average value of the data points or the interpolated data points that have the same theta angle among the sector.

Click the up or down arrows of the “Azimuthal Angle (deg.)” or the “Sector Width (deg.)” input box, the values in the input box, the blue lines, and the profile curve will change simultaneously.

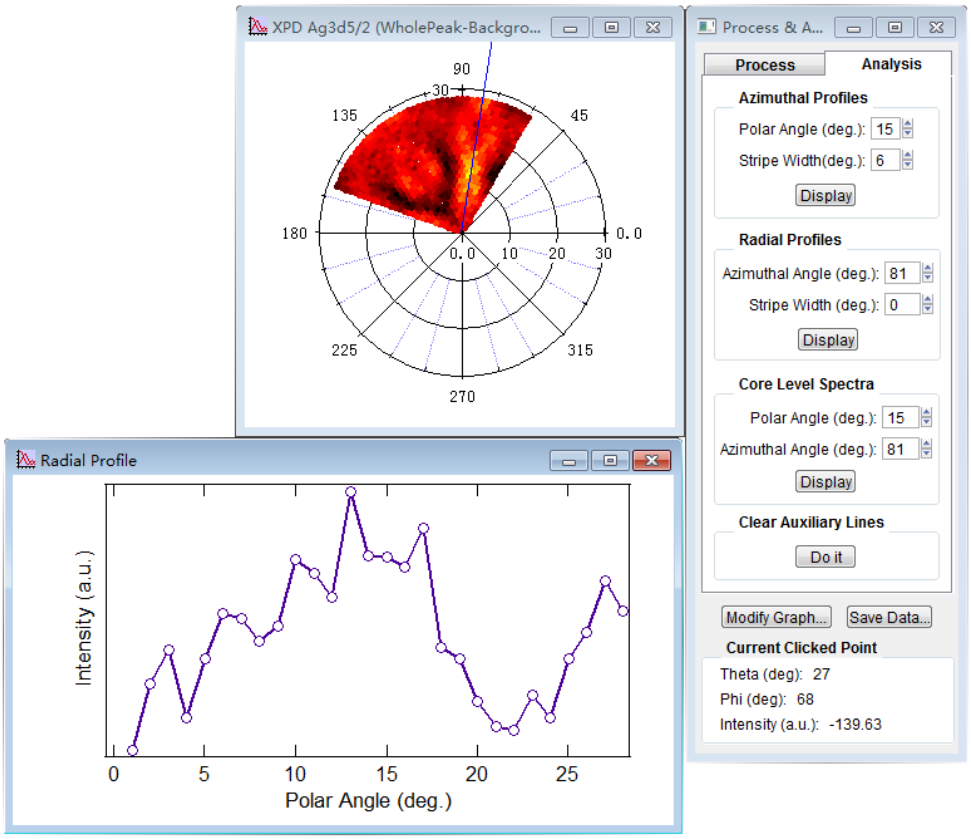



Fig. 21. A blue line shown on the pattern (Sector Width = 0) and the corresponding radial profile curve displays in a graph window.

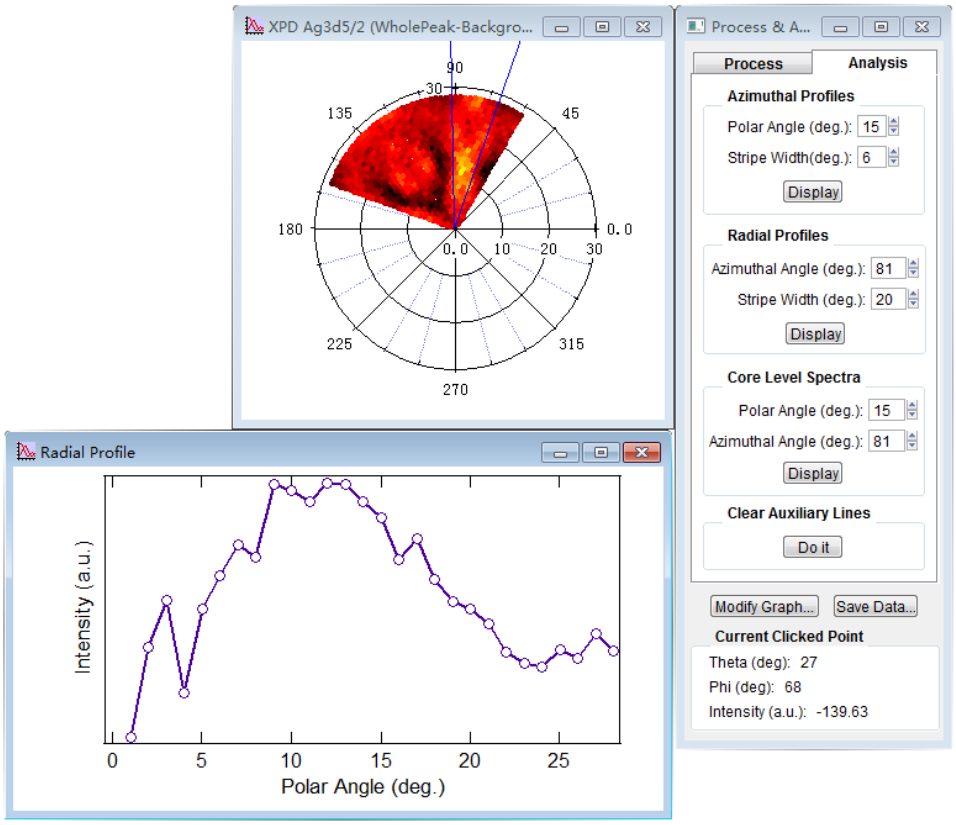



Fig. 22. Two blue lines shown on the pattern (Sector Width > 0) and the corresponding radial profile curve displays in a graph window.

### 5.3. Display the core-level spectra of a selected data point

Click the “Display” button in the "Core-level Spectra" group box, the corresponding core-level spectra of a specified data point will display in a “Core-level Spectra” graph window (Fig. 23).

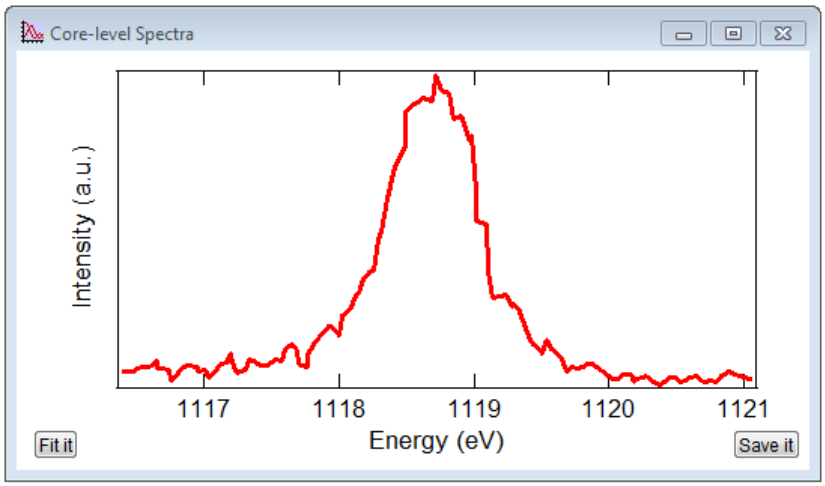



Fig. 23. The core-level spectra window.

### 5.4. Fit a core-level spectrum

Click the "Fit It" button at the bottom-left corner of the core-level spectra window, the IGOR's built-in MultipeakFit window will pop up and let users do multi-peaks fitting to this spectrum (Fig. 24). Please refer to IGOR Pro's help manual for detailed information about the usage of MultipeakFit.

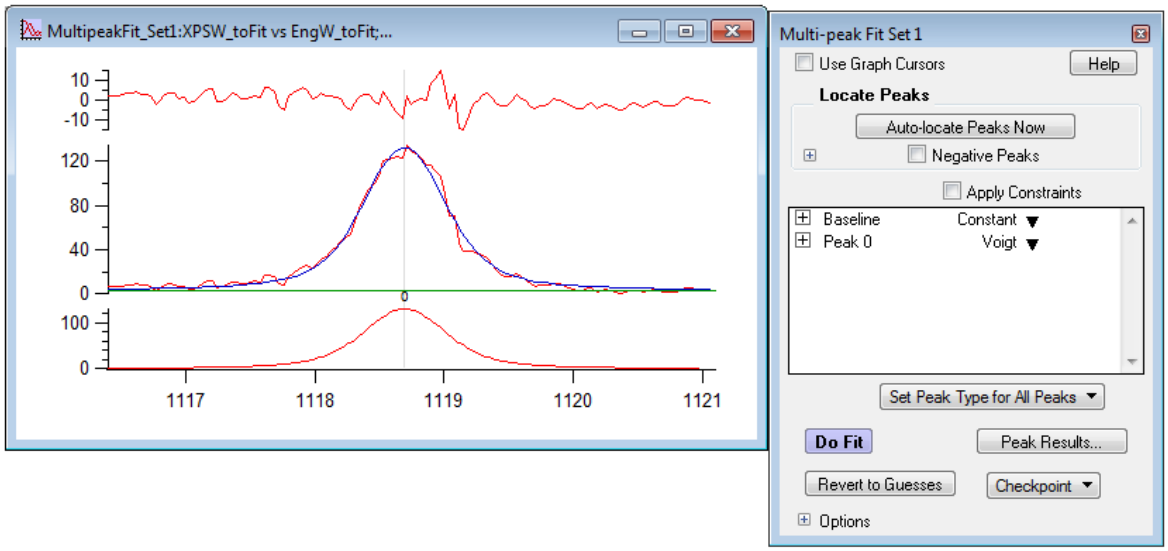



Fig. 24. The IGOR's built-in MultipeakFit window.

### 5.5. Save the data of a spectrum

Click the "Save it" button at the bottom-right corner of the Core-level Spectra window (Fig. 23), users can save the data of displayed spectrum to a text file (*.xy) for future processing.

### 5.6. Modify a pattern's appearance

Right click a pattern and select "modify polarY0" in the right-click menus, a "Modify Trace Appearance" window (Fig. 25) will pop up and let users to change the pattern's appearance. For example, click the "Set as f(z)…" button, the "Set as f(z)" window (Fig. 26) will pop up. Choose the "Color Table" to change the color map of the XPD pattern. The color map in Fig. 12 is YellowHot, and it can be changed to Terrain as shown in Fig.27.

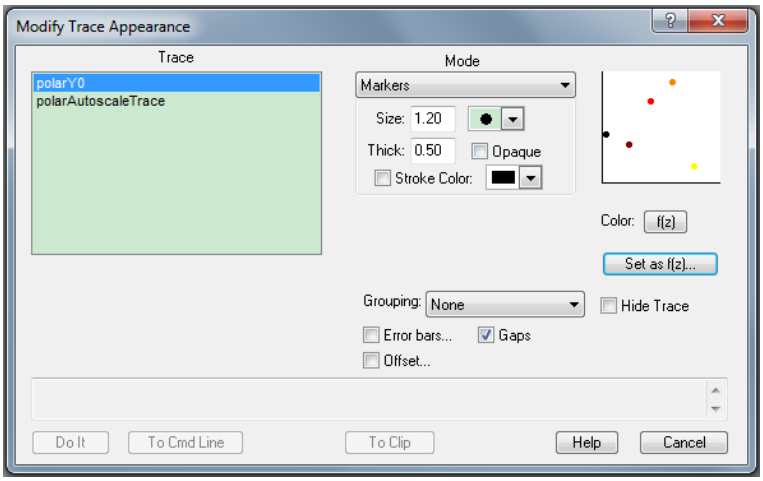



Fig. 25. The “Modify Trace Appearance” window.

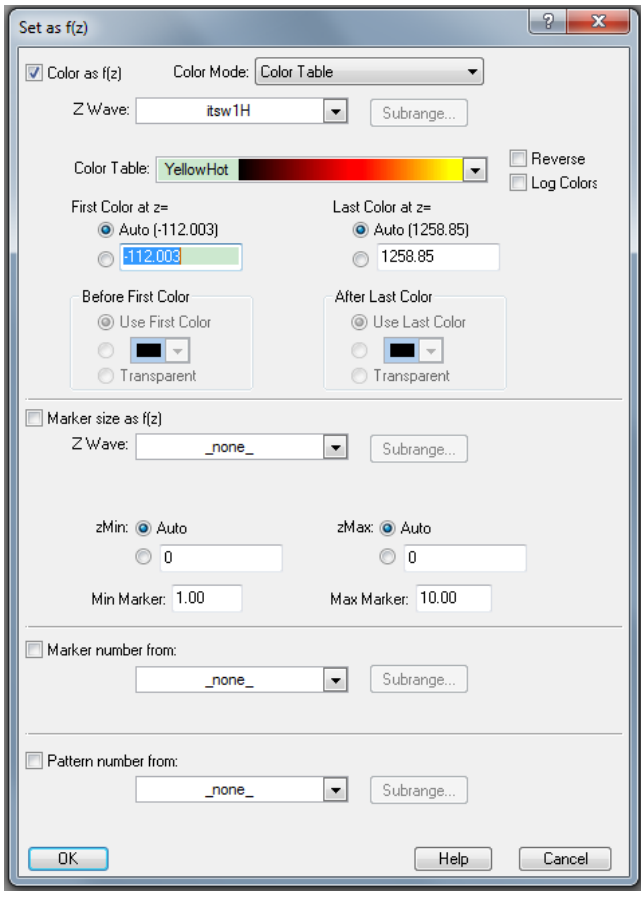



Fig. 26. The “Set as f(z)” window.

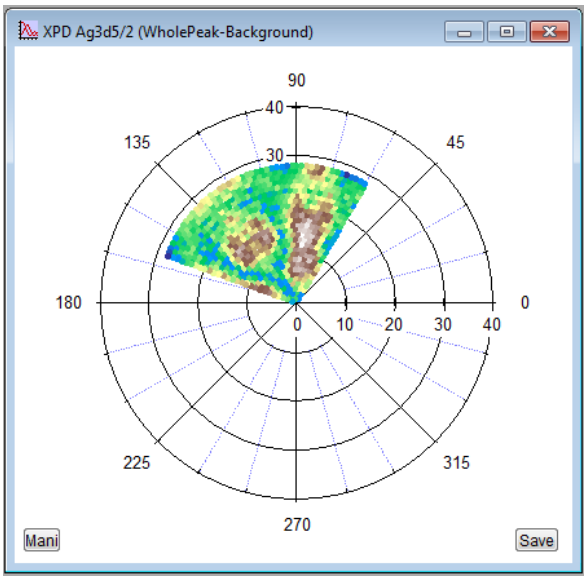



Fig. 27. The XPD pattern in Terrain color map.

### 5.7. Modify a graph's properties

Click the "Modify Graph..." button, a Polar Graphs setting panel (Fig. 28) will pop up to let users change a graph's properties. The Range, Axes, Ticks, and Labels of the XPD pattern graph can be changed. Please refer to IGOR Pro's help file for detailed information about the usage of the Polar Graphs setting panel.

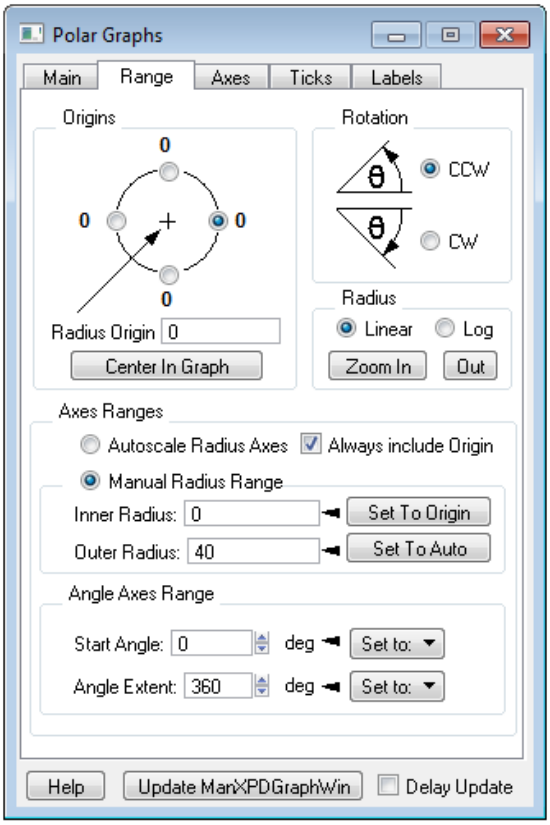



Fig. 28. The Polar Graphs setting panel.

**6. Open an XPD pattern**

Click the "Open a diffractogram" in the XPD menu (Fig. 2) to open an XPD pattern for processing and analysis. The data file must have been saved by this package and its extension name is ".xpd".

**7. Generate series of variable step size scan angles**

Clicking on the 'Generate angle scan files' submenu will open the 'Generate Angle Scan Files' panel (Fig. 2) for generating series of variable step size scan angles.

The azimuthal steps at different polar angles are varied according to azimuthal equidistant polar projection method. The calculation method of azimuthal variable step size is detailed in Appendix A.

**8. Import dispersion factors**

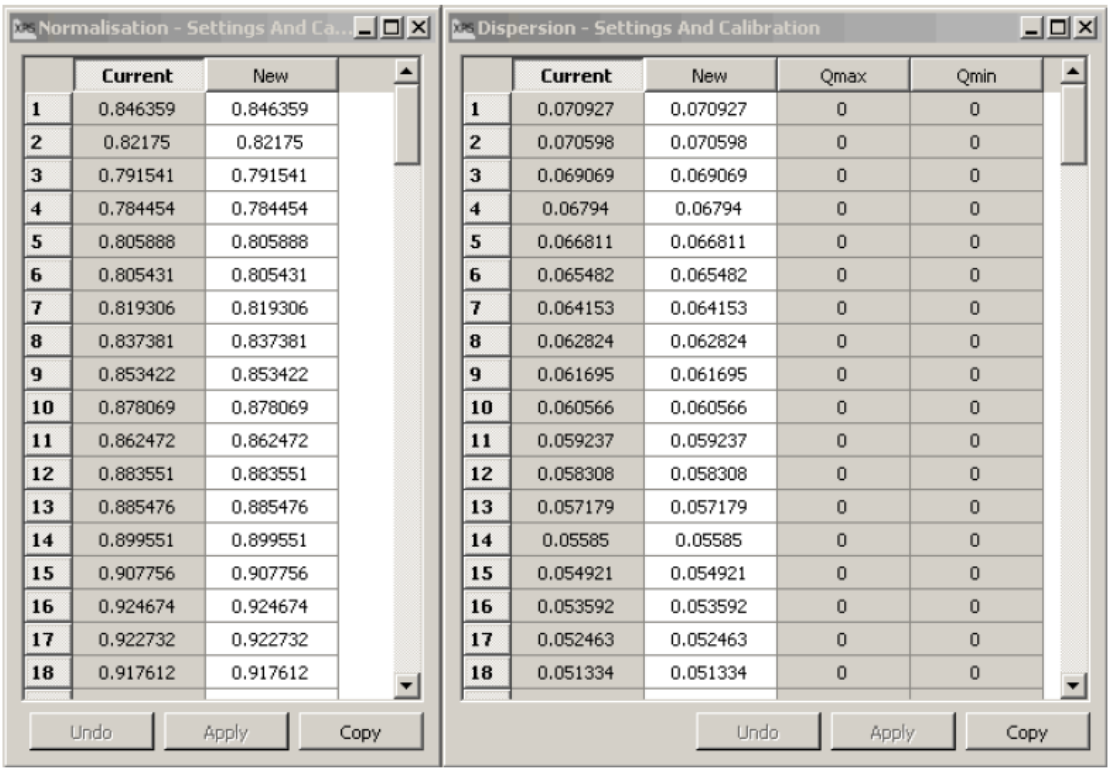
Because the raw XPS data saved by the Omicron software (i.e. MATE script of the MATRIX in our case) is not calibrated for the XPD system in CEA photoemission lab, the XPD package needs the dispersion factors to calibrate the photoelectron intensity of each channel of the Omicron Argus analyzer's detector.

The dispersion factors are saved in the package once imported, so the 'Import Dispersion Factors…' menu is rarely used except that it's the first time to start acquisition via the 'XPD Data Acquisition' panel after the installation of the package or that the dispersion factors of the analyzer's detector have been recalibrated.

Clicking the "Import Dispersion Factors…"menu will bring up an open dialogue for users to select a dispersion factors file for importation. The dispersion factors should be saved in a text file beforehand. Below is the method how to create a dispersion factors file in the Omicron MATRIX, which is in the Page 8 of Omicron MATRIX Update Manual as shown in below.

- In the *Normalisation* window select the *Current* row and copy the data to the clipboard (<CTRL>-C) or use *Copy* button. Open an ASCII editor (e.g. Notepad) and paste the data into the editor. Save the values to a text file (e.g. NormalisationValues.txt).

- Do the same with the *Current* row in the *Dispersion* window and save these data into a separate file (e.g. DispersionValues.txt).



Normalisation - Settings And Ca...

| | Current | New |
|---|---|---|
| 1 | 0.846359 | 0.846359 |
| 2 | 0.82175 | 0.82175 |
| 3 | 0.791541 | 0.791541 |
| 4 | 0.784454 | 0.784454 |
| 5 | 0.805888 | 0.805888 |
| 6 | 0.805431 | 0.805431 |
| 7 | 0.819306 | 0.819306 |
| 8 | 0.837381 | 0.837381 |
| 9 | 0.853422 | 0.853422 |
| 10 | 0.878069 | 0.878069 |
| 11 | 0.862472 | 0.862472 |
| 12 | 0.883551 | 0.883551 |
| 13 | 0.885476 | 0.885476 |
| 14 | 0.899551 | 0.899551 |
| 15 | 0.907756 | 0.907756 |
| 16 | 0.924674 | 0.924674 |
| 17 | 0.922732 | 0.922732 |
| 18 | 0.917612 | 0.917612 |

Undo Apply Copy

Dispersion - Settings And Calibration

| | Current | New | Qmax | Qmin |
|---|---|---|---|---|
| 1 | 0.070927 | 0.070927 | 0 | 0 |
| 2 | 0.070598 | 0.070598 | 0 | 0 |
| 3 | 0.069069 | 0.069069 | 0 | 0 |
| 4 | 0.06794 | 0.06794 | 0 | 0 |
| 5 | 0.066811 | 0.066811 | 0 | 0 |
| 6 | 0.065482 | 0.065482 | 0 | 0 |
| 7 | 0.064153 | 0.064153 | 0 | 0 |
| 8 | 0.062824 | 0.062824 | 0 | 0 |
| 9 | 0.061695 | 0.061695 | 0 | 0 |
| 10 | 0.060566 | 0.060566 | 0 | 0 |
| 11 | 0.059237 | 0.059237 | 0 | 0 |
| 12 | 0.058308 | 0.058308 | 0 | 0 |
| 13 | 0.057179 | 0.057179 | 0 | 0 |
| 14 | 0.05585 | 0.05585 | 0 | 0 |
| 15 | 0.054921 | 0.054921 | 0 | 0 |
| 16 | 0.053592 | 0.053592 | 0 | 0 |
| 17 | 0.052463 | 0.052463 | 0 | 0 |
| 18 | 0.051334 | 0.051334 | 0 | 0 |

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**Appendix A: Calculation of azimuthal variable steps size**

The two widely used planar projection methods in XPD experiment are azimuthal equidistant polar projection (AEPP) and stereographic projection (SP). It's very convenient to use AEPP in IGOR Pro, below is the calculation of azimuthal variable steps size for AEPP.

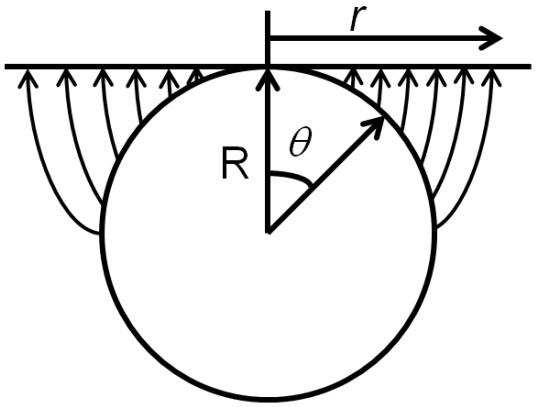


Fig. A1. AEPP method.

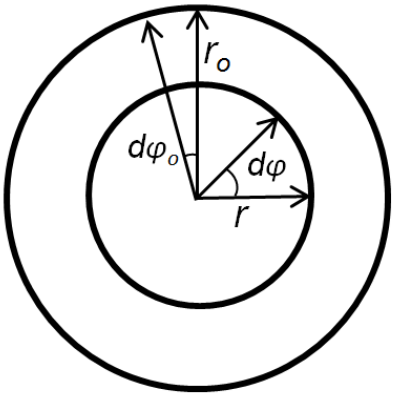


Fig. A2. A projection plane.

Briefly, in AEPP, the equal increments in the polar angle ($\theta$) are presented by equal increments in the radial direction in the projection plane (see Fig. A1). Therefore, if the radius in the plane is $r$, and the radius of the sphere is $R$, then

$$r = R*\theta,$$

Here the unit of the $\theta$ is radian.

If the radius of the outmost circle is $r_o$ (corresponding polar angle is $\theta_o$), the radius of any other circle is $r$ (corresponding polar angle is $\theta$), the azimuthal step size of the outmost circle is $d\varphi_o$ (the initial step in the XPD package), the azimuthal step size of any other circle is $d\varphi$ (see Fig. 2). The pixel density of the two circles on the projection plane should be equal, *i.e.*, the distance between the two adjacent data points of the two circles should be equal:

$$r*d\varphi = r_o*d\varphi_o\,,$$

$$R*\theta*d\varphi = R*\theta_o*d\varphi_o\,,$$

So,

$$d\varphi = d\varphi_o*(\theta_o/\theta).$$

For example, if the polar angle of the outmost circle is $80^o$ ($\theta_o$) and the initial azimuthal step size is $1^o$ ($d\theta_o$), then the azimuthal step size ($d\varphi$) of the circle whose corresponding polar angle is $20^o$ ($\theta$) is

$$d\varphi = 1^o * [(\pi*80^o/180^o)/(\pi*20^o/180^o) = 4^o$$