

Data Collection on XPERT XRD with new X'celerator Detector

Slit Settings

Only two slits are used for the new detector. A divergence slit (S1) and an anti-scatter slit (S2). Because the resolution is determined mostly by the pixel size of the detector, using smaller slit does not necessarily improve the resolution. Several settings with typical applications are listed below

S1	S2	Intensity (%)	Resolution (Deg)	Comments
1	2	100	0.10	Recommended for most powder & thin film samples
1/2	1	55	0.08	Use this only if resolution is important
1/4	1/2	28	0.08	Do not use this!
1/16	1/8	N/A	N/A	Use this only for SAXS measurements. Minimum 2Theta is 0.5 deg.

Starting Data Collector

1. Start DATA COLLECTOR program and log in
2. Click 'INSTRUMENT' ->'CONNECT'
3. In list of configurations, choose 'X'celerator & PRS', and click 'OK'
4. Click 'OK' in pop up information window. Once instrument is online, control panel is located on the left of the window.
5. From the menu on the top, choose 'CUSTOMIZE -> OPTIONS', and in the pop up window, click on 'POWDER' and choose configuration to be 'X'celerator & PRS'. THIS STEP IS NECESSARY ONLY FOR THE FIRST TIME YOU LOG IN.
6. In control window, click on 'INCIDENT BEAM OPTICS' tab
7. Click on 'Divergence Slit' (Slit #1 in instrument) and 'Anti-scatter Slit' (Slit #2) and change to the values of slits used in the instrument. (Recommended: 1 deg for Divergence Slit and 2 deg for Anti-scatter slit). DO NOT CHANGE OTHER SETTINGS.
8. Click on the tab 'Diffracted Beam Optics' and click on 'Detector..'. In the pop up window, choose

Type: X'celerator[2]

Usage: Scanning

Active Length (2 Theta): 2.122

Click 'OK' to close window

Manual Scan

1. In control window, click on 'INSTRUMENT SETTINGS', then 'POSITIONS' to open up a pop up window showing current positions of the instrument. Type in desired position and click 'APPLY' or 'OK' to move the instrument
2. Choose 'MEASURE' => 'MANUAL SCAN'
3. In the parameter window, change 'Range' and 'Time/Step' to set up the scan. DO NOT CHANGE 'STEP SIZE (0.0083556)' AND 'SCAN SPEED'

4. Click 'OK' to start the scan. Data will be displayed in a graphics window. A green line representing the resting position of the instrument once the scan is finished.
5. Right click in the graphics window to choose 'ZOOM', 'PEAK', 'FWHM' modes for the display
6. Choose, 'FILE' =>'Save As' to save data to your own folder
7. Click 'OK' to close manual scan window

Program Scan

1. On the file menu, choose 'NEW PROGRAM'. Choose program type and click 'OK'
2. In the program set up window, choose scan type (Gonio for default), type in 'START ANGLE' and 'END ANGLE'. DO NOT MODIFY STEP SIZE AND TIME
3. Click on 'SETTINGS' to open another window with list of all the instrument parameters. Most of them will show 'ACTUAL'. From the list, click on 'Detector', on the window below, choose

Type: X'celerator[2]

Usage: Scanning

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4. Click 'OK' to return to the main program window, which will show a step size of 0.0167113. DO NOT MODIFY STEP SIZE AND SCAN SPEED. Change 'TIME/STEP' to set total scan time.
5. Click on 'x' to close and save the program
6. On the menu, choose 'MEASURE -> PROGRAM'. Select correct folder and type in dataset name. Click 'OK' to start data collection. Data will be saved automatically.

Data Printing

Use the program DATA VIEWER to display and print data

Data Processing

Use the program HI-SCORE to display, treat, index, and match the diffraction data to known phases contained in PDF 2 database. Refer to quick start manual for HI-SCORE located on the desktop for details.

Pole Figure/Texture Measurement

At this point, the configuration for measuring pole figure data using the new detector has not been determined. If you have a need to do texture scans, please contact Youli Li to set up the instrument.

Data from Old Computer

All scan data from the old computer had been converted to the new format and are located in the folder c:\X'PERT_Data\Converted xpert32 under different user names.