

The following illustrates how to execute the fit2d using non-graphical mode in the command-line style. While the square represents the return key and bold words have to been input manually

hooknose:/net/cci/jyan/fit2d % **fit2d -key -nogr**

PROGRAM FIT2D Version: V12.081

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FIT2D: 2-D Detector Calibration/Correction; File re-formatting; 2-D Fitting

YOU CAN ALWAYS ENTER: ?
FOR FURTHER EXPLANATION OF REQUIRED INPUT

No commercial software used !
Readline replaced, now escape key works !
Mar image plate data vertical ordering reversed !

See "CHANGES" (keyboard menu) for important changes

INFO: The graphics system has been turned off by a command line option

X DIMENSION FOR ARRAYS (Range: 1 to 1000000) [3450]:

Y DIMENSION FOR ARRAYS (Range: 1 to 1000000) [3450]:

CREATE VARIANCE ARRAYS [NO]:

Main menu: ENTER COMMAND [INPUT DATA]:

FILE FORMAT [FIT2D STANDARD FORMAT]: **mar research format**

NOTE: USING NEW INPUT CODE

DATA FILE NAME [no_data.dat]: **LaB6.mar3450**

INFO: Image size = 3450 3450 Number of overloaded pixels = 1101

INFO: The following information has been extracted from the file header:

Date and time of scan = Sat Nov 5 20:

Sample to detector distance = 100.00 mm

Wavelength is = 1.5418 Angstroms

Phi angle at the start of the oscillation = 308.497 degrees

Phi angle at the end of the oscillation = 309.497 degrees

(These values may be changed using the "GEOMETRY" command.)

Main menu: ENTER COMMAND [IMAGE]: **fit**

Fit sub-menu: ENTER COMMAND [INPUT PARAMETERS]: **powder diffraction**

INFO: The current pixel coordinates for the beam centre = 1753.732 1565.734

INFO: The current pixel sizes (microns) = 100.000 100.000
INFO: The current sample to detector distance (millimetres) = 100.000
INFO: The rotation angle of the tilt plane = -59.554
INFO: The tilt angle of the detector = -0.717

CHANGE BEAM CENTRE AND/OR TILT VALUES [NO]: **yes**

X-PIXEL COORDINATE OF BEAM CENTRE [1753.732]:

Y-PIXEL COORDINATE OF BEAM CENTRE [1565.734]:

X-DIRECTION PIXEL SIZE (MICRONS)

(Range: 1.000000E-03 to 10000.00) [100.0000]:

Y-DIRECTION PIXEL SIZE (MICRONS)

(Range: 1.000000E-03 to 10000.00) [100.0000]:

SAMPLE TO DETECTOR DISTANCE (MILLIMETRES)

(Range: 0.100000 to 1.000000E+05) [100.0000]:

TILT PLANE ROTATION ANGLE (DEGREES)

(Range: -180.0000 to 180.0000) [-59.55398]:

DETECTOR TILT ANGLE (DEGREES) (Range: -180.0000 to 180.0000)
[-0.717304]:

CORRECT FOR X-RAY BEAM POLARISATION [YES]:

BEAM POLARISATION (AT SAMPLE) (Range: -1.000000 to 1.000000)

[0.990000]:

Ready for input of Lorentz Geometry

TYPE OF LORENTZIAN CORRECTION TO APPLY

[PARTIAL POWDER (2-THETA SCAN)]:

PRODUCE EQUAL ANGLE PIXEL SCAN [YES]:

2 THETA SCAN ANGULAR PIXEL STEP (DEGREES)

(Range: 1.000000E-03 to 10000.00) [5.700000E-02]:

TAKE ACCOUNT OF SPATIAL DISTORTION [NO]:

INFO: Starting to re-bin 2-D data to a 1-D profile, this can take some
time for large arrays.

INFO: Number of rows treated = 300 (8%)

INFO: Number of rows treated = 600 (17%)

INFO: Number of rows treated = 900 (26%)

INFO: Number of rows treated = 1200 (34%)

INFO: Number of rows treated = 1500 (43%)

INFO: Number of rows treated = 1800 (52%)

INFO: Number of rows treated = 2100 (60%)
INFO: Number of rows treated = 2400 (69%)
INFO: Number of rows treated = 2700 (78%)
INFO: Number of rows treated = 3000 (86%)
INFO: Number of rows treated = 3300 (95%)

INFO: Minimum fractional intensity decrease owing to polarisation = 0.2534
INFO: (The reciprocal value is applied to the data.)

SAVE DATA IN "POWDER DIFFRACTION STANDARD" FORMAT [YES]:*no*

Fit sub-menu: ENTER COMMAND [EXIT]:

Main menu: ENTER COMMAND [EXCHANGE]:

Main menu: ENTER COMMAND [IMAGE]:*output data*
FILE FORMAT [FIT2D STANDARD FORMAT]:*gsas*

OUTPUT FILE NAME [LaB6.gsas]:

OUTPUT ROWS [YES]:

NUMBER OF ROW TO OUTPUT (Range: 1 to 1) [1]:

Main menu: ENTER COMMAND [INPUT DATA]:*exit*
CONFIRM EXIT [NO]:*yes*

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      FFFFFFF      T      22      D
      FFFF      TT      2222      DD
      FFFF      I      TT      22 22      DD
      FFF      II      TTT TTT 22 22      DDD
      FFF      FF I      TTTTT 2 222      DDD
      FFFF FFFF I      TTTTTT 2 222      DDD
      FFFFFFFF      II TTTTTTTT 2 222      DDDDDD
      FFFFFFFF      II TT TTT      222      DDD DDD
      FF FFF      III      TTT      22      DD DDD
      FFF      II      TTT      22      DD DDD
      FFF      II      TTT      22      D DDD
      FF      II      TT      22      D DDD
      FF      II      TT      2222      DDDDDD
      F      I      T      222222222222      DDD
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INFO: BYE: FIT2D V12.081 exited by user command

INFO: (No commercial software is used within FIT2D.)
Spline surface fitting uses FITPACK, written by Paul Dierckx

hooknose:/net/ccl/jyan/fit2d %