RADFN

v1.12

1. Introduction

RADFN is an fiber diffraction program designed for measuring intensity data from partially oriented specimens. With X-ray diffraction data on a polar grid, the program performs background subtraction, disorientation deconvolution, and overlapping correction, to extract the intensity for each reflection on the grid. RADFN is based on an angular deconvolution algorithm and procedure described in this paper: Makowski, 1978, J. Appl. Cryst., 11, 273-283.

2. Input

RADFN reads diffraction data files in "polar reciprocal for angular deconvolution" format produced by WCEN where all data corrections (such as polarization, fiber tilt and twist) should have been applied. Input data files contain two sections:

2.1. Header

IFV: if layer lines are vertical, 0 for no, 1 for yes.

NULB: data discarded if its bad pixel count exceeds NULB. not currently used.

RMIN: the radius (measured in WR) of the first annulus, where the data begins. this depends on the lower resolution bound you chose in data transformation in WCEN.

NR: total number of annuli.

WR: width of annulus in pixels, corresponding to the x/rad bin size in WCEN).

DR: pixel size (mm/pixel).

XWAV: x-ray wavelength.˚

THMIN: starting angle of annuli, usually 0˚.

DTHET: bin size along an annulus, usually 1˚.

NTHET: number of bins in an annulus, usually 91 (0˚ to 90˚).

AME/BME: file names. not currently used.

IFOG: 1 if fog has been subtracted. not currently used.

NGEOM: 1 if geometric calculations have been applied. not currently used.

IOPT: 1 if non-linearity corrections for optical density have been applied. not currently used.

IQ: quadrants used (0 or 1 for each of 4 quadrants). not currently used.

SFD: specimen to film/detector distance in mm.

REPEAT: repeat distance of diffracting molecule.

2.2. Data

There are NR sets diffraction data, each containing NTHET entries (usually 91, 0º to 90º inclusive). The first number in each entry is the number of bins along the annulus. The second is intensity. The third is the number of pixels in the bin, or number of bad pixels in the bin. The last number is the standard deviation of the pixel intensities in the bin. The last two numbers are not currently used in RADFN.

3. Output

RADFN can output raw deconvolution data with statistics, or diffraction amplitudes only, in 0.001Å intervals along each layer line, interpolated from raw data.

A raw output file contains two sections.

The first section shows the background information associated with each annulus you have processed, and the second section lists the intensity information contributed by each annulus for each layer line. For the first section, the first column is the radius (of an annulus), the second is the background (which should be changing smoothly), the third is the second background, if applicable, and the fourth (or the third if one background) is the error.

For the second section, the first column is layer line number, the second is R, the third is the amplitude, the fourth is the radius, the fifth is D*, the distance along the radius in reciprocal space, the sixth is the position where the layer line was predicted to be, the seventh is the shift in degrees of the calculated from the predicted, and the last column the layer line width (in degrees).

4. Main Menu

4.1. File Menu

Open: open a diffraction data file. only polar reciprocal format is currently supported.
Save: save angular deconvolution data into a file.

Exit: exit the program.

4.2. Option Menu

Plot: change the color scheme for plotting.
Output: choose interpolation method for deconvoluted data.

4.3. Tools Menu

Background: plot and smooth background data obtained by angular deconvolution.

4.4. Window Menu

Input File: display the input file in a text editor.
Pattern: display the diffraction pattern and the annulus currently being processed.
Log: display work done thus far.

4.5. Help Menu

About: program information and credit

5. Control Panels

5.1. Run Panel

Init: initialize angular deconvolution.

CurrR: process the current annulus, specified on right.

NextR: process the next annulus (current + 1).

Integ: integrate 1 or more peaks instead of fitting.

Cut: cut off data beyond a degree, specified on right (if 0, RADFN will decide where to cut).

Uncut: go back to the uncut fitting of the data.

Summa: show summary of processed annuli.

5.2. Input Panel

The parameters on this panel are picked up by RADFN from the header of the input file. User needs to verify the correctness of the values.

XWAV: x-ray wavelength.

SFD: specimen to film/detector distance in mm.

C: repeat distance of diffracting molecule.

DR: pixel size (mm/pixel).

WR: width of annulus in pixel (x/rad bin size in WCEN).

IFV: if layer lines are vertical, 0 for no, 1 for yes.

NULB: data discarded if its bad pixel count exceeds NULB. not currently used.

RMIN: the radius (measured in WR) of the first annulus.

NR: total number of annuli.

THMIN: starting angle of annuli, usually 0.

DTHET: bin size along an annulus, usually 1.

NTHET: number of bins in an annulus, usually 91 (0 to 90).

5.3. Param Panel

This panel contains control parameters for angular deconvolution. User must check each value and make appropriate changes.

NREFIN: rounds of refinements to fit the calculated to the observed intensities.

NPR: 1 if peak positions are to be found before refinement of peak heights, otherwise they are done together.

MAXLLS: maximum layer line shift in degrees. RADFN will search [-MAXLLS, MAXLLS] by a step of MAXLLS / 5.

MINCUT: lower bound for automatic cut.

XINT: increment to usual upper integration limit (half way between layer lines).

BGINT: 1 if to use local background in integration, 0 for global.

INTL: 1 if local background to be taken from only one point at the limit of integration, instead of the average of this point and its two outer neighbors.

NBKGD: number of background terms, 1-5:

1: constant k (almost always used).
2: constant k + funny term, now obsolete, like cos.
3: two possibilities:
F (Fourier series): k + k1.cos(t) + k2.cos(2t)
G: k + funny term + meridional Gaussian
4: k + k1.cos(t) + k2.cos(2t) + k3.sin(2t)
5: k + k1.cos(t) + k2.cos(2t) + k3.sin(2t) + k4.sin(t)

where t is the azimuthal angle theta on the pattern. Use of 4 and 5 is not recommended.

BK2: 0 for Gaussian, 1 for Fourier.

BK3: 0 for Gaussian, 1 for Fourier.

CENGB: 90 for meridional Gaussian (for modeling slit scatter).

SIGMON: half-width of BK2/BK3 if it is Gaussian

5.4. Gauss Panel

The layer line cross-sections are defined here.

IG: number of Gaussians representing layer line cross-section:
1: cross section is a Gaussian (default), for well-oriented specimens.
2: cross-section is two Gaussians, slightly offset, for single quadrant.
3: cross section is a Gaussian, with two more Gaussians equal in height to each other, offset equal distances on opposite sides of the main Gaussian. This is used when there is a second oriented domain in the specimen causing a second, slightly shifted diffraction pattern. It is 3 rather than 2 because of the effect of averaging quadrants.

If IG is set 2 or 3, the followings need to be specified:

SIGG: half-width of Gaussian, essentially the disorientation

SIGG2: half-width of the second Gaussian if exists

DCEN: the separation between the two Gaussians in degrees

GRAT: relative intensity of the second Gaussian to the first

6. Plot

The plot shows the fit between the calculated and the observed intensities. The white dots represent the observed intensity on the annulus, from 0-90˚ (from equator to meridian). The red

tick marks at the bottom appear every 10˚. The horizontal red line shows the global background. The green vertical lines are where peaks found on that radius. The yellow vertical lines are where the layer lines would be according to fiber repeat. White vertical lines indicate that data near the meridian are so distorted that RADFN can't fit them; instead, it does an integration.

The data near the meridian is not as accurate as the data close to the equator where sampling is finer. At the meridian, the R distance between two points in an annulus is much greater. Also, disorientation at the meridian smears data across layer lines, while at the equator, smearing is within layer lines.

7. Running RADFN

1. Open an input file (File -> Open)
2. Set up parameters on control panels
3. Initialize angular deconvolution (Run panel -> Init)
4. Process annuli
5. Save output