This program is developed for polychromatic x-ray diffraction of polycrystalline samples. Major capabilities include:

(1) Simulate diffraction pattern of a given material

(2) Calculated radially averaged 1D diffraction profile from 2D diffraction data from APS 32-ID-B beamline.

(3) Index (hkl) of diffraction data

Data to load:

*.tif (series) files, *tiff file or converted *.mat files

*.txt file for energy spectrum (first column energy, second colomn flux)

*.txt file for absorption (first column energy, second colomn transmission)

Basic parameters:

(1) Sample-to-detector distance: from sample to detector plane

(2) Detector angle: angle between detector plane surface normal and incident beam

(3) Pixel size: assuming square pixel shape

(4) Scaling factor: data binning factor, used for accelerating analyis speed

(5) Image dimension: pixel numbers of the detector

(6) Number of harmonic peaks: how many harmonic energies users would like to consider when labeling the (hkl) peaks

(7) Direct beam X and Y (optional): direct beam position on detector, could be negative number. If not known, users can use "Find (00)" tool to estimate them.

(8) Content in "Sample structure" module: weight of diffraction intensity of each phase in the overall diffraction pattern. This is not the mass or mole content, instead, it's simply a parameter to for data fitting. Without input, the default is 50% for each.

(9) Points in "Tools" module: Number of point for scattering vector q in I(q) (and I(tth)) plots.

(10) Q res in "Tools" module: half width of q window when performing radially average. The larger the number, the smoother the intensity profile. It should be equal or slightly larger than the half of the difference of adjacent q points.

Sample structure information:

Users need to input sample crystal structure and reference diffraction information for using "Simulate diffraction" and "Label (hkl)" tools.

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