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DEBYE

Simulation program for powder diffraction
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Reference:
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General:
The Debye simulation program calculates the XRPD pattern from a crystalline sample by summing over all interatomic distances as stated by the Debye equation (Debye, 1915, Ann. Phys. 46: 809). The crystallographic information can be imported from a cif and modified if necessary. Additional information about particle shape, size and size distribution can be supplied. The min, max and step in 2theta as well as the wavelength can be altered to agree with experimental XRPD data. Finally the simulated data can be convoluted with a polarisation function, a pseudo-Voigt type instrument profile (Wertheim et al., 1974, Rev. Sci. Instrum. 45(11): 1369) and functions related to the Guinier diffraction geometry and absorption in cylindrical samples.

Thermal parameters:
The program only works with isotropic thermal parameters, and these are averaged to one per atom type. If the crystallographic information read from a cif does not contain a Biso, it will be calculated from the anisotropic thermal parameters in case these are given, otherwise the program defaults to Biso=0.

Limitations:
The program is presently limited to five different atom types.

GUI:
The Windows GUI for the Debye program offers the opportunity to open an experimental XRPD pattern, simulate or open an earlier simulated diffractogram for comparison, and do a fit. The progress of the simulation and fitting can be followed in the lower text window while the diffraction patterns are shown in the upper graphical window. It is possible to zoom in the graphical window by holding down the left mouse button and dragging a window of the desired size.

Fitting:
During the fitting procedure the simulated diffractogram is scaled using either an ordinary scale factor, an overall temperature factor, or both. The background is modelled as a Chebyshev polynomial with a user-specified number of parameters (between 0 and 14). A 2theta zero shift can be manually added during the fitting procedure.
The fitted parameters and their standard deviations are written on the rec file (see files below) and can be viewed via patterns, table output.
Based on the fitted background it is possible to calculate the crystallinity, the fraction of intensity resulting from the simulated crystalline part of the sample, between any two values of 2theta.
N.B. The crystallinity calculation is only valid if the background represents amorphous scattering from the sample only.

How to install:
Copy debye.exe and DebyeHelp.txt (this file) into
a common directory and make the appropriate correction to the

winpow.ini file to define the default directory and the path leading to notepad.exe or some other text editor.

Files:
To do the simulations a name.rec input file in ascii format is needed. The input file can be constructed from scratch using the commands listed below. It is, however, much easier to import the crystallographic information from a cif and define the desired structural parameters via the GUI menus. If an experimental diffraction pattern is imported for fitting it is possible to obtain the following output files:

%name.out	List file summarising the simulation
%name.tab	Tabulated summary of simulation and fitting
%name.xy	Simulated diffractogram
%name.sum	2theta, experimental pattern, simulated and fitted pattern, difference, background.
%name.fdp	Pair distribution function. Only for the first atom type.

Multiple simulations:
For more time-consuming calculations the Debye program offers the opportunity to run a series of simulations without having to start each simulation manually in the GUI. For this purpose all the rec files must first be constructed along with a file called "anything.mlt" containing the names of all the rec files to run, one name per line, eg:
name1.rec
name2.rec
name3.rec
Under file, open project choose the mlt file and select project, calculation.

Shortcut keys:

up arrow	Zoom out in graphical window
down "	Zoom in "
left "	Move zoom window left
right "	Move zoom window right
F1	Return graphical window to full view
F2	Return graphical and text windows to original size
F3	Project, calculate
F4	Patterns, fit pattern
F5	File, save project as
F6	Project, edit files
F7	Project, edit structure
F8	Project, edit instructions
ctrl-T	Patterns, table output

List of records in the name.rec input file for the Debye simulations:

Required records:

SPGR Space group symbol in the old Hermann-Mauguin notation with inversion centre at origo, e.g. P 21 21 21, P -3, P 63/M, F d d d. For rhombohedral space groups use the hexagonal setting.

CELL Cell dimensions

11-20	cell(1)	a [A]
21-30	cell(2)	b [A]
31-40	cell(3)	c [A]
41-50	cell(4)	alpha [deg]
51-60	cell(5)	beta [deg]
61-70	cell(6)	gamma [deg]

XYZ Atomic coordinates

11-14	atomname	Atom identifier
18-20	atype	Atomic number
21-30	x	Fractional coordinates

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      31-40  y               "
      41-50  z               "
      51-60  sof         Site occupancy factor
      61-70  Biso        Isotropic temperature factor coefficient B=U8PI**2


Optional records:

TITL  11-78  Title of the job

PWDT  11-70  Name of experimental diffraction pattern file

FRMT  Input data format (optional)
      11-15              1 – gdf (Huber)
                         2 - txt (Bruker)
                         3 - udf (Philips)
                         4 - xrdml (PANalytical)
                         5 - xy (general)
                         6 - std (general)

ELAM  Wavelengths (default: 1.54059, 0, 0 - CuKalpha1)
      11-20  lambda(1)   [A]
      21-30  lambda(2)   [A]
      31-40  lambda(3)   lambda2/lambda1 intensity ratio

ANOM  Anomalous dispersion corrections (defaults to MoKalpha,
      CuKalpha or CoKalpha depending on which wavelength is
      closest)
      11-14  atomname    Atom identifier
      21-30  fp          f'
      31-40  fpp         f''

DDIS  Distance calculation accuracy (default: 100)
      11-20  disacc      Reciprocal of the distance
                         calculation accuracy [A-1]

DSHA  Particle shape (default: 1, 3)
      11-15  crysttype   1 – box
                         2 – cylinder
                         3 - ellipsoid
      16-20  cylaxis     1 – a*
                         2 – b
                         3 – a*xb

DABC  Particle size
      If crysttype = 1: number of cells along the a-, b- and c-axis
      (default: 10, 10, 10)
      If crysttype = 2: cylinder dimensions [A]
      (default: 100., 50.)
      If crysttype = 3: ellipsoid dimension [A]
      (default:    50., 50., 50.)
      11-20  ncella/cyllen/ellips1
      21-30  ncellb/cylrad/ellips2
      31-40  ncellc/ellips3

DPSD  Particle size distribution (PSD) (default: 0, 3, 1)
      11-15  ptype        0 – do not apply PSD
                          1 – apply PSD
      16-20  psample      number of sizes sampled on
                          either side of the mean (max 9)
                          NB! Only sizes 1.0+-0.1 psample,
                          eg. 0.8, 0.9, 1.0, 1.1 and 1.2
                          times the input size (psample=2)
      21-25  distype      1 – Weibull mass distribution
                          2 – Gaussian      "
                          3 – Uniform       "
                          4 – User defined  "
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DUS1  User defined mass distribution coefficients
      required for distype=4 (default: 0.,...,0.)
      11-20  puser(-9)    mass fraction of particles
      21-30  puser(-8)    with a size defined as
      31-40  puser(-7)    0.1, 0.2, 0.3, 0.4 etc times the input size
      41-50  puser(-6)
      51-60  puser(-5)
      61-70  puser(-4)
      71-80  puser(-3)

DUS2  User defined mass distribution coefficients
      11-20  puser(-2)
      21-30  puser(-1)
      31-40  puser(0)
      41-50  puser(1)
      51-60  puser(2)
      61-70  puser(3)
      71-80  puser(4)

DUS3  User defined mass distribution coefficients
      11-20   puser(5)
      21-30   puser(6)
      31-40   puser(7)
      41-50   puser(8)
      51-60   puser(9)

DTTH  2theta interval information and scale factor
      (default: 5., 50., 0.02, 0)
      11-20  ttmin       2thetamin  [deg]
      21-30  ttmax       2thetamax  [deg]
      31-40  ttdif       2thetastep [deg]
      41-50  ttsca       =0 – intensity per unit cell is output
                         >0 – intensity output for ttsca
                              unit cells
                         <0 – simulated pattern will be
                              scaled to Imax=-ttsca

DCOR  Intensity corrections (default: 1, 0, 0, 0, 0, 1.)
      11-15  corrpol     0 – no polarisation correction
                         1 – polarisation correction
      16-20  corrpeak    0 – no instrument profile
                         1 – pseudo-Voigt instrument peak
                             profile correction
      21-25  corrabs     0 – no absorption correction
                         1 – correct for absorption in
                             cylindrical sample
      26-30  corrguin    0 – no guinier correction
                         1 – correct for 45 deg Guinier
                             tangent angle
      31-35  corrauto    0 - no auto divergence slit
                         1 - auto divergence slit correction
      36-45  corrmur     value of muR for absorption correction

DPRO  pseudo-Voigt peak profile parameters (gL+(1-g)G)
      (default: 0., 0., 0.01, 0.5, 0., 0.)
      11-20  uu          FWHM
      21-30  vv          (Caglioti et al., 1958, Nucl. Instrum.
      31-40  ww          Methods 3(4): 223)
      41-50  g1          pseudo-Voigt mixing parameter
      51-60  g2          g = g1+g2(2theta)+g3(2theta)2
      61-70  g3          (Hill and Howard, 1985, J. Appl. Cryst.
                         18(3): 173)


Records added by the fitting routine:

SCAL  Scale factors (default: 1., 0.)
      11-22  scal        scale factor from fitting
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      23-32  ovrl        overall temperature factor

ZETT  2theta zero shift (default: 0.) NB! Not refined
      11-20  zett        2theta zero shift

BKGR  Chebyshev background parameters (default: 0.,...,0.)
      NB! Three records, 0-14 Chebyshev parameters
      11-20  bkg1/bkg6/bkg11
      21-30  bkg2/bkg7/bkg12
      31-40  bkg3/bkg8/bkg13
      41-50  bkg4/bkg9/bkg14
      51-60  bkg5/bkg10

DCRY  Crystallinity (default: 5., 50., 0.)
      11-20  crystttmin  [deg]
      21-30  crystttmax  [deg]
      31-40  xtallinity  Crystallinity calculated
                         between crystttmin and crystttmax

DVAL  Fitting results
      11-20  fitpatrval  Pattern R-value from fit
      21-30  fitpatwrval Weighted pattern R-value
      31-40  fitpatgof   GooF from fit
      41-47  fitpatnpar  Number of fitted parameters
      48-54  nstep       Number of 2theta steps
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