Manual of the JAVA frontend of eCMWP

all lengths are in units of nanometer [nm]

CUBIC, HEXAGONAL, ORTHOROMBIC

click the appropriate crystal structure

lat_a, lat_b, lat_c,

put in the corresponding lattice constants
for cubic or hexagonal leave lat_b and lat_c, or lat_b empty, respectively

Burgers vector

here you can insert the Burgers vector of dislocations
for hexagonals or orthorombics this will be a "formal" values which will have to be "re-evaluated" once the patterns have been done

Wavelength

here you can insert the wavelength you are using
when neutron diffraction patterns are worked on you have the option to use d*=1/d=K
in such a case you have to click: "Fit in K instead of 2*theta:" below

Ch00 or Chk0:

when average dislocation contrast factors can be used you can insert the
$\bar{C}_{h00}$, or $\bar{C}_{hk0}$ values for cubic or hexagonal crystals, respectively
for more details see: *J. Appl. Cryst. (1999). 32, 992-1002, Powder Diffraction 17 (2), June 2002*, or *J. Appl. Cryst. (2002). 35, 556-564*

Don't include size effect:

if you are sure that in your pattern there is no size-effect, you may click here,
however, it is better to set "init_b" to 10 and "init_c" to 1, and "fix" these two values, see more to these two parameters below

Use ellipsoidal size func.:

if you suspect that your coherently-scattering-domains are better approached as "rotational ellipsoids" than spheres you may click here
in such a case the "init-epsilon" becomes active

Use individual C factors:

when you suspect that for any reason the average dislocation contrast factors are not appropriate, you may click here, in such a case the values in "Ch00" or "Chk0" become irrelevant; when this option is activated the value of "init_d" will not be changed and the dislocation density provided in this case can only be considered as a "formal" value; for more details see: *Nature, 428 (2004) 837-440, Scripta Materialia 63 (2010) 69–72, Materials Science and Engineering A 528 (2010) 112-121*,

Include St.Fault effect:

if you suspect or have indications that your specimen does contain planar defects, i.e. twin boundaries, or other kind of planar defects, like intrinsic or extrinsic stacking-faults, you can click here, at the same time you have to connect the appropriate "stacking,dat file" by using the "Browse" button, the "stacking,dat file"-s are free to download using the CMWP homepage, for details see: *J. Appl. Phys. 100 (2006) 023512, J. Appl. Crystallogr. 42 (2009) 580–591*.

stacking,dat file

see the item before,

Use weights:

when there are very large differences in the intensity-maxima of the different reflections, e.g. of the order of 10^2 or 10^3, you may click here, the peaks will be weighted, within a certain 2θ or d* range, by the reciprocal of the square of the intensity maxima of the profiles, you have to bare in mind that weighting will also change the emphasis of the different peaks as the contribution to the entire evaluation, the effect of weighting can be assessed by inspection of the fitting quality by using the "View FIT" button,

Disable coinc. g^2 code:

when working on single-crystals you may have profiles with the same d* values but corresponding to different orientations, in this case you can evaluate these profiles simultaneously, however, you must apply this button, along with this it is advisable to apply the "Use individual C factors:" option,

Use instrum. profiles:

for instrumental corrections you have to apply this button, at the same time you have to include the directory consisting of the appropriately prepared instrumental profiles, for this you have to use the "Browse" for the "Instrum. profile dir" position, for more details see the manual of CMWP or the phd-work of Ribarik, both free to download from the CMWP homepage,

Fit peak int.:, Fit peak pos.:

the CMWP procedure is not refining the unit cell, therefore, both the peak intensities and the peak positions are "free" parameters in the entire procedure; since the initially determined peak intensities or positions may not have been the ideal values for the fitting of the physical profiles functions, both the peak intensities and the peak positions can be adjusted by clicking these two buttons; the two can be activated simultaneously or sequentially according the your own decision,

Fit in K instead of 2*theta:

if the pattern is given in $K=2\sin\theta/\lambda=d^*$, this button has to be activated; this option is especially useful for neutron diffraction patterns measured in TOF mode;

Clone peak-index.dat file:

when a series of patterns are evaluated where the peak positions and intensities do not change considerably, this button can be used to import already existing peak-index.dat files,

Clone bg-spline.dat file:

when a series of patterns are evaluated where the background does not change considerably, this button can be used to import already existing bg-spline.dat files,

FT limit (if no instr.eff.):

when the instrumental effect is negligible and there is no need for instrumental correction the smallest value of the FT has to be limited; the default value is 10^{-7};

Profile cutting parameter:

the theoretical profile functions will be calculated for the first indexed Bragg reflection in the $\Delta K=2[\sin(\theta+\theta_0)/\lambda - \sin(\theta-\theta_0)/\lambda]$ range, where $2\theta_0$ is the Bragg angle of the first indexed Bragg reflections and $\theta-\theta_0$ is the value of the cutting parameter; all higher angle reflections will be evaluated within the same ΔK range; the appropriate value of the "cutting parameter" depends on the broadening of peak profiles; it should be large enough in order to include the "tail" parts into the evaluation, however, if real "background" is involved into the evaluation the iterations may become unnecessarily long,

N1; N2:

these are the number of sampling within the range determined by the "cutting parameter" and in-between, respectively; latter throughout the entire pattern; sometimes it might be useful to change this number to 512, especially if the software does not start working despite no obvious error,

Min. 2*theta/K, Max. 2*theta/K:

these are the 2θ or K range of the patterns; the gnuplot figures will be displayed in this range during the evaluation procedure,

Fit limit:

the evaluation procedure is controlled by the weighted-sum-of-squared-residuals (WSSR), when the relative decrease of the WSSR reaches the value of "Fit limit" the procedure will stop automatically; the default value is 10^{-9},

Fit. max. num. of iter.:

this is the number of iterations after which the procedure will stop, irrespective of the "Fit limit" value,

init_a(CUB):

this is the q parameter in the average dislocation contrast factors for cubic crystals, if "CUBIC" is active at the top of the frontend, for starting the procedure there must be a number here, for details see *Phys. Stat. Sol. (a), 171 (1999) 425-434*,

init_a1(HEX|ORT), init_a2(HEX|ORT):

these are the a_1 and a_2 parameters in the average dislocation contrast factors for hexagonal or orthorhombic crystals, if "HEXAGONAL" is active at the top of the frontend, for starting the procedure there must be numbers here, for details see *Phys. Stat. Sol. (a), 171 (1999) 425-434, J. Appl. Cryst., 35 (2002) 556-564, phd-work of Ribarik*,

a_fixed:, a1_fixed:, a2_fixed:

if the pattern is not good enough to provide physically reasonable values for these parameters you may fix the values you think are more appropriate, and the other physically relevant parameters can still be determined,

init_a3(ORT), init_a4(ORT), init_a5(ORT):

these are the a_3, a_4, and a_5 parameters in the average dislocation contrast factors for orthorhombic crystals, if "ORTORHOMBIC" is active at the top of the frontend, for starting the procedure there must be numbers here, for details see the *phd-work of Ribarik*,

a3_fixed:, a4_fixed:, a5_fixed:

if the pattern is not good enough to provide physically reasonable values for these parameters you may fix the values you think are more appropriate, and the other physically relevant parameters can still be determined,

init_epsilon:

if you think that the size of the "coherently scattering domains" in your specimen are anisotropic in specific crystallographic directions, you may click here, and your size broadening will be evaluated by assuming that the "coherently scattering domains" are rotational ellipsoids in specific crystallographic directions, the default value here is l, meaning shape-isotropy, for details see the *phd-work of Ribarik*,

epsilon_fixed:

if you wish, you may fix the initial value of "epsilon", in this case it will not be changed during the procedure,

scale_a, scale_b, scale_c, scale_d, scale_e:

the five parameters, a, b, c, d and e can be "scaled", in the numerical procedure the scaled values are considered, however, the corresponding physical values are calculated by taking into account the "un-scaled" parameter-values, for a, b and c the best scaling is unity (1), for d and e the best scaling is 100 and 0.01, respectively,

init_b:

the median, i.e. the m parameter in the logarithmic-normal size distribution function is: m=exp(b), in that sense b is the initial value for the "median", b=2 or 3 are typical values for "nanocrystalline" size values, b=7 or larger means practically that there is "no size effect" in the pattern,

b_fixed:

here you may fix the value of b, in this case it will not change during the procedure,

init_c:

the logarithmic-variance, i.e. the σ parameter in the logarithmic-normal size distribution function is: $\sigma=c/\sqrt{2}$, in that sense c is the initial value for the " logarithmic-variance", c=0.1 or 0.2 are typical values for practically "monodisperse" size distribution, c=1.5 or larger means "very wide" size distribution, a variety of average size-values can be obtained as the different moments of the logarithmic-normal size distribution function, since the TEM micrographs are the image of a thin planar section of the material, the size obtained from a TEM images is in best correlation with the second momentum of the logarithmic-normal size distribution function, i.e. the area average crystallite size: $<x>_{area}=m\times\exp(2.5\times\sigma^2)$, e.g. with c=1.5 $<x>_{area}=m\times16.65$, for more details see *Powder Diffraction, 20 (2005) 366-375,*

c_fixed:

here you may fix the value of b, in this case it will not change during the procedure,

init_d:

the dislocation density, ρ is related to d as: $\rho=2/\pi/(b_{BV}\times d_{scaled})^2$, where b_{BV} is the Burgers vector, this means that ρ is proportional to $1/d^2$, when d is "scaled" with 100, a good initial values is 2, note that when "Use individual C factors:" is active the initial value of d will not be changed during the procedure,

d_fixed:

here you may fix the value of d, in this case it will not change during the procedure, this need not be activated when "Use individual C factors:" is active, it is also noted that fixing of d is not advised, see "d*e_fixed" below,

init_e:

the effective outer cut-off radius of dislocations, R_e is related to e as: $R_e^*=(e^{-1/4})/(2\times e_{scaled})$, for the meaning of the asterisk see M*, when e is "scaled" with 0.01, a good initial values is 2,

e_fixed:

here you may fix the value of e, in this case it will not change during the procedure, it is noted that fixing of e is not advised, see "d*e_fixed" below,

init_st_pr.:

here you can give the initial value for planar defect density in percentage, when activating this option the "stacking,dat file" must be filled up appropriately by browsing,

stacking_pr_fixed:

here you may fix the value of "init_st_pr.", in this case it will not change during the procedure,

d*e_fixed:

if the pattern is not good enough to determine the appropriate value of the effective outer cut-o ff-radius of dislocations, R_e, this is the right option to interfere interactively, the absolute value of R_e itself depends on the absolute value of the dislocation density, ρ, itself, therefore Wilkens introduced the dimensionless, physically more appropriated value of $M=R_e\sqrt{\rho}$, [*M. Wilkens, in: J.A. Simmons, R. de Wit, R. Bullough (Eds.), Fundamental Aspects of Dislocation Theory, vol. II., Nat. Bur. Stand. (US) Spec. Publ.*

No. 317, Washington, DC, USA, 1970, p. 1195.], M is the "arrangement parameter" of dislocations, for details see also *Materials Science and Engineering A 528 (2010) 112–121*, since the value of M depends on both, R_e and ρ, the control of M can only be done correctly if the product d×e is controlled, this is done by fixing d*e, it is important to note that the physically appropriate M value is: $M=e^2\times M^*\cong 7.4\times M^*$, when $M\leq 1$ the dislocation arrangement is strongly of "dipole character" when $M\geq 1$ the dipole character is less strong, $M\geq 5$ is almost as if it would be infinite, all these statements are rather qualitative, if a series of patterns are evaluated with the purpose of determining the change of dislocation densities and it can be assumed that the "dislocation arrangement" does not change during the process investigated it might be advisable to control the value of M (or M*) within a certain range, $\pm\Delta M=10\%$ (or $\pm\Delta M^*=10\%$) will not effect the change in the dislocation density considerably, if, however, $\pm\Delta M\geq 10\%$ (or $\pm\Delta M^*\geq 10\%$) the mere fluctuations in the M or M* values may produce unnecessary fluctuations in the dislocation-density values, when the value of $d_{scaled}\times e_{scaled}=4$, M* will be $M^*\cong 0.35$ and $M\cong 2$, which are medium reasonable values,

Number of phases:

there is the option to evaluate more than one phase simultaneously, in such a case here you have to put in the number of phases,

Select phase to edit:

when more than one phase is evaluated the second or more phase initial values will have to be edited separately and this button has to be filled up appropriately by activating the "Edit selected phase" button,

Call MKSpline, Call MKSpline2,

this activates the background spline adjustment, see also the *phd-work of Ribarik*, without the background spline the procedure will not start,

Call MKSpline2

when stopping the procedure by having activated "**Stop FIT**" you may activate here; a gnuplot window will pop-up with the measured, the fitted and the background patterns in green, red and blue; using the left-button on your mouse you may adjust the background-spline in order to bring the measured and calculated patterns closer to each other; this option allows subtle corrections to the background; note that the default intensity scale is logarithmic, this means that the lower intensity values and the background itself are strongly enlarged compared to the rest of the pattern,

Index peaks

this activates an auxiliary program for indexing and positioning the peaks and produces the "peak_index.dat" file, without such a file the procedure does not start, see also the *phd-work of Ribarik*,

Set individ. C values:

this activates an auxiliary JAVA frontend where the individual dislocation contrast factor values can be edited,

Clone INI files:

when starting with a new pattern which has more-or-less the same structure and initial values as a pattern which was already evaluated, you can import the old "initial" values by using this button,

Save INI files:

this saves the initial values used in the evaluation

(Re)Start FIT:

here you can start or re-start the evaluation procedure,

Stop FIT:

at any moment of the evaluation procedure it can be stopped/halted when pressing here, a "promt window" will appear showing the progress of stopping "gnuplot", please wait until the last iteration is stopping, after that you can work in the JAVA frontend again,

Update params:

if you wish, you can update the parameter values to the ones actual at the end of the last iteration, if you restart the procedure it will continue with the actual values appearing in the JAVA frontend,

View solutions:

with this a "promt window" can be opened where you can view the solutions obtained by the last iteration before the procedure was stopped, this window stays open until you close it yourself,

Exit:

here you can leave the evaluation,

Comment

the procedure produces a fairly large number of auxiliary files, the two most useful for the user are the *.sol (the larger one) and the *.int4.dat files; the *.sol file consists of all input and output data and results corresponding to the last evaluation; the *.int4.dat file is a 4 column text file with the 2θ (or K) values, the measured, the calculated intensities and the difference values, this file can be used for plotting the pattern and the evaluation in any graphic program; if, during the evaluation procedure, you have stopped and restarted the procedure you can see the results of each intermediary evaluation by entering: your actual CMWP directory and going to "results/evaluate-int-dir/*.*

forum:

with further questions/comments/suggestions you may contact: ungar@ludens.elte.hu or ribarik@renyi.hu