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Appendix
Computing Diffraction Contrast

Algorisms

The computing formulas come from the books, “electron Microscopy of thin crystal”(1965), which is based on papers published in early 1960s by

Howie and Whelan, and "Diffraction and Imaging Techniques in Material Science" (1978) in Howie' s chapter.

1. Howie/Whelan's scattering matrix supposition

Intensity=uu* (u and u' are the wave amplitude at opposite of the slab)

$u'=\boldsymbol{P}u$ (1)

$\boldsymbol{P}$ is the scattering matrix.

$\mathbf{P}=\mathbf{C}\{\exp(2\pi\gamma^{(i)}dz)\}\mathbf{C}^{-1}$

For the nth slab,

$\mathbf{P}n=\mathbf{Q}^{-1}{}_n\mathbf{P}\mathbf{Q}_n$

$\boldsymbol{P}=\mathbf{P_1}\ \mathbf{P_2}\ \mathbf{P_3}\cdots\ \mathbf{P_n}$

$\mathbf{Q}n=\{\exp(2\pi\mathbf{g.R})\}$

C is the matrix whose columns are the eigenvectors of equation:

$\mathbf{A}\mathbf{C}^{(i)}-\gamma^{(i)}\mathbf{C}^{(i)}=0$ need derivate the eigen

A is matrix whose diagonal elements are

$\mathbf{A}_{00}=0+1/\ \xi_0'$, $\mathbf{A}_{gg}=\mathbf{s}_g+1/\ \xi_0'$

And whose off-diagonal elements

$\mathbf{A}_{gh}=1/2\xi_{g-h}+1/\ 2\xi_{g-h}'$

2. Howie's Differential equation of interband and intraband scattering of Bloch waves

$d\Psi\ /dz=2\pi i\{e^{-2\pi i\gamma(i)z\ }\}C^{-1}\ \{\beta_g'\}C\ \{e^{2\pi i\gamma(i)z}\ \}\Psi$ (2)

Ψ is Boch wave excitation.

$v=C\{e^{-2\pi i\gamma(i)T\ }\}\Psi$ T=foil thickness

Intensity=vv*

3. Howie/Whelan's Direct integration of wave vectors

$dv/dz=2\pi i\{A+\ \{\beta_g'\}\}v$ (3)

Intensity=vv*

4. Howie/Takagi many beam wave formula

$d\Phi_g\ /dz=\pi i\Sigma\{\Phi_{g-g'}e^{-2\pi i[(sg-sg')z+(g-g').R]}(1/\xi_{g-g'}+i/\xi_{g-g'})\}$ (4)

Intensity=ΦΦ*

Equations (1) and (2) need solve the eigen values.

Equations (2)-(4) are treated using the explicit Runge-Kutta method.

The four equations described above build the foundation to simulates the diffraction contrast
of dislocations under many-beam (weak beam) conditions. The column approximation used
makes it very easy to use the power of multiple-core CPU. Each time, a CPU(core) is used to
calculate the intensity from a column, which means N-times faster than using a single
computer (N= the number of CPU(cores) used). Matrix operation (derivation of eigen values,
matrix inverse etc.) is driven by LINPACK. The explicit Runge-Kutta method of order 5 is the default
integrator DOPRI5 (Hairer, Norsett and Wanner 1993, C++ version by Blake Ashby).
A stiff integrator (C++Radau5) is selectable.

The displacement field was from FORTRAN codes A. Head et al (1973).
d(g.R)/dz→d(g.R)/dy =
1/2π∑{(x*c1-
c2*b2)*b3/(b4*b4+(y+b2)*(y+b2))+c2*b3*(y+b2)/((y+b2)*(y+b2)+b4*b4)}
(for equations (2) and (3))
Z and Y have a simple geometrical relation described in configuration.
This stress field was formulized by A Head based on the analytical model by Stroh.

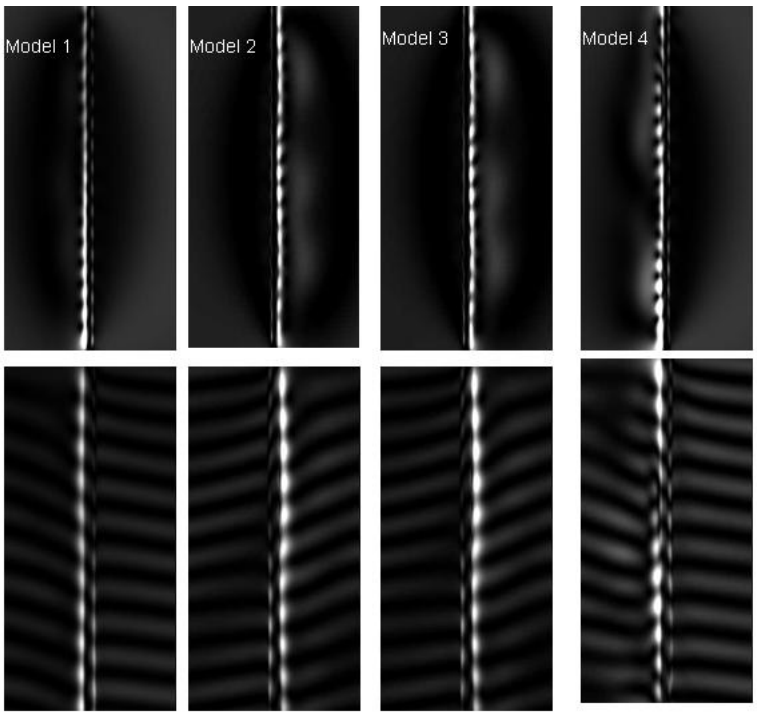
It is a straight solution to obtain
g.R=1/2π∑ (x*c1-
c2*b2)*b3/b4*atan((y+b2)/b4)+c2/2*b3*log((y+b2)*(y+b2)+b4*b4);
by d(g.R)/dy=f(y) g.R=∫ f(y) dy
(for equations (1)+(4)).

Test results:
Using a quad-core CPU (suse linux) system

	Model 1	Model 2	Model 3	Model 4
Speed (time spent in mins) Uniform thick (60 nm)	7.2	4.9	13.5	36.7
Speed (time spent in mins) wedge (20-60 nm)	5.6	3.4	10.1	21
Apparent fault spacing in nm for uniform thickness	4.6(11 pixels)	5 (12 pixels)	5(12 pixels)	4.6(11 pixels)

Comparison in dislocation contrast

Contrast from Shockley partials (copper)



Contrast from super-partials (Ni3Al)

Contrast from stack faults