Multislice simulation of CBED patterns

Andrey Chuvilin and Ute Kaiser

Universität Ulm, Materialwissenschaftliche Elektronenmikroskopie, Albert Einstein Allee 11, 89069 Ulm, Germany

http://www.uni-ulm.de/elektronenmikroskopie/mattem/

Motivation for using MS for CBED calculations

Bloch Wave (BW) method is used for calculations of CBED patterns from perfect crystals however cannot be applied for the case of imperfect crystals without further approximation.

Advantages of MS are:

no column approximation
- CBED for the structures with high strain gradient and for irregular structures (structure defects, interfaces, statistically distributed point defects, etc) can be directly calculated;

no independent plane waves approximation
- position sensitive coherent CBED patterns can be calculated for regular and irregular structures;

calculation speed
- large disordered models can be calculated at reasonable time.

We acknowledge the valuable discussions with Prof. M. Tanaka, Prof. K. Tsuda and Dr. A. Preston.
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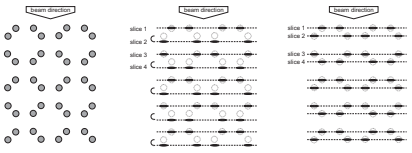
Requirements for MS for CBED simulations

Sampling in real space - to calculate HOLZ line with **g**-vector of **G**nm^{-1}, the phase grating should sampled at least as 1/(2**G**)nm, which gives 0.01nm for typical **g**-vectors of HOLZ lines of about 50nm.

Sampling in reciprocal space is determined by a desired resolution of HOLZ lines. In order to image a line (~0.05nm^{-1} wide) with at least 2 pixels, the sampling interval should be 0.025 nm^{-1}. This determines the supercell size in real space to be at least 40nm.

Full 3D symmetry rather than 2D projection symmetry of the crystal must be preserved in calculations in order to reproduce HOLZ lines positions and intensity correctly.

Modification of a slicing scheme in order to preserve 3D symmetry



Crystal structure

Equal slice thickness.
3D symmetry is lost.

Unequal slice thickness.
3D symmetry is preserved.

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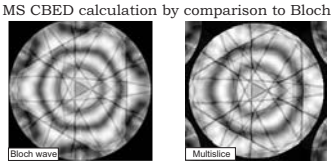
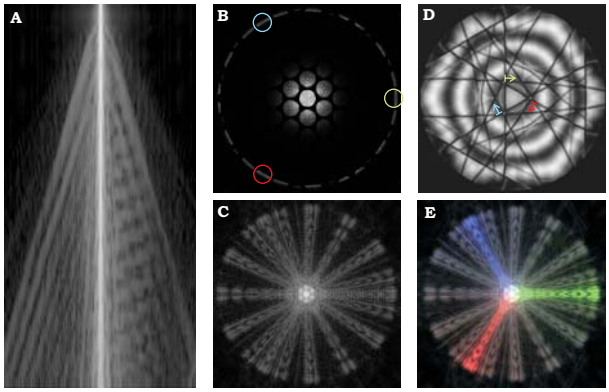
Validation of MS CBED calculation by comparison to Bloch waves CBED.



Si [111], 100 kV, scattering potentials according to [P.A. Doyle, P.S. Turner, Acta Cryst. A 24 (1967) 390-397] , Debye-Waller factor - 0.003 nm^2, absorption - 0, supercell for MS - 40x40 nm^2, matrix - 4Kx4K, probe diameter - 0.3nm.
HOLZ lines position and intensity correspond well in both cases. MS by 2% overestimates the thickness in comparison to BW.

Peculiarities of CBED pattern formation revealed by multislice simulation



Multislice calculation enables to establish direct relation between real and reciprocal features of CBED.

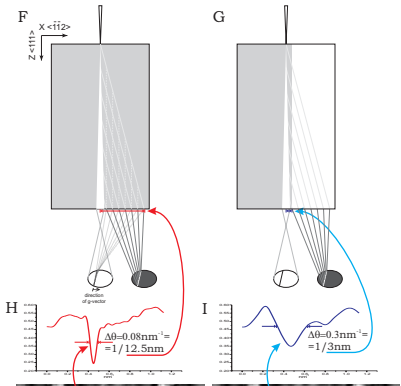
A. Scattering to their Bragg angles (typically 5-15 deg) HOLZ lines cover significant area on the exit surface of the sample.

B. MS simulated CBED pattern of Si [111] 100kV at 210nm thickness.

C. Wave in real space (log scale of intensity) at the exit surface of the sample, corresponding to the diffraction at B. Intensity corresponding to HOLZ lines is spread 20nm away from the central beam. The actual value for the size of scattering region is determined by $\Delta r = T * tg(2\Theta)$, where Θ is a Bragg angle of corresponding HOLZ reflection and T is a sample thickness.

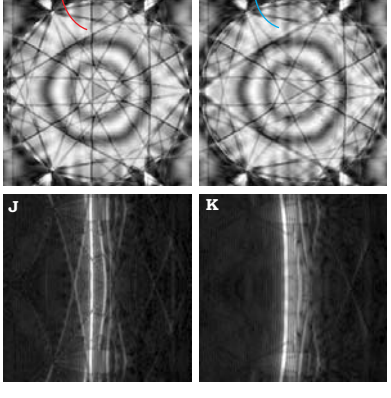
D. Central disk of B. Arrows indicate directions of g-vectors of <-11 5 5> reflections.

E. Image C overlayed with colour coded dark field images calculated for HOLZ reflections marked at B and D. Each of the reflections has its particular lengthy scattering region.



F. Scheme for the bulk crystal model and HOLZ line scattering.

G. Scheme for the crystal with the edge and HOLZ line scattering in this case.



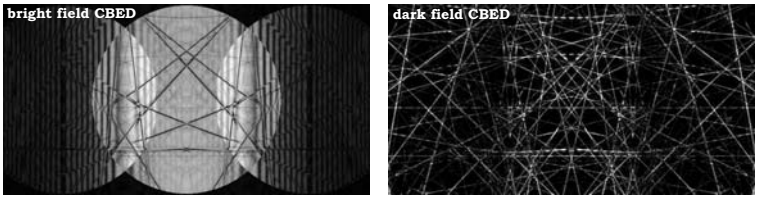
H, I. Central disks of simulated CBED patterns for both cases and profiles of intensity of affected **deficient** HOLZ line. The width of deficient lines is determined by the whole scattering region of the lines. Lines with g-vectors pointing along or away from the edge stay unaffected.

J, K. Corresponding **excessive** lines. Note dynamical shape of the line (X-section of dispersion surface) for the bulk case (**J**), and kinematical shape (X-section of Ewald sphere) in the case of an edge (**K**). Note, that width of excessive lines do not differ significantly.

Take-home-message:
In contrary to the assumption made by the column approximation, central CBED disk combines structural information from different stretched regions around the central beam.
The position and the shape of deficient HOLZ lines are determined by the scattering conditions in the regions where they propagate, rather than the conditions at the position of the beam.

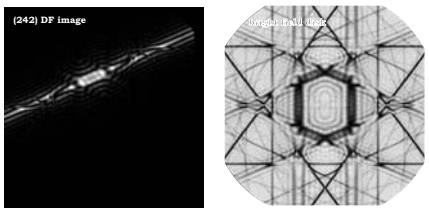
What can be done with MS calculations?

Dark field CBED calculations
(see for example M.Tanaka et. al., JEM, 33(3) (1984) 195-202)

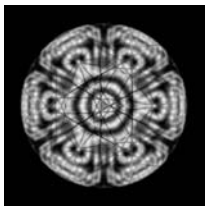


Si[331], 100kV, thickness 237nm

LACBED calculations

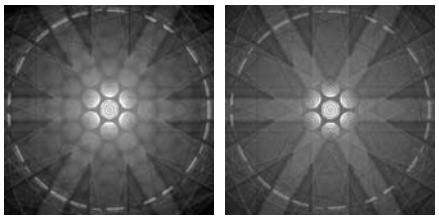


AlInAs[012], 300kV, thickness 120nm
(joint work with D. JACOB, LSPES UMR CNRS France)



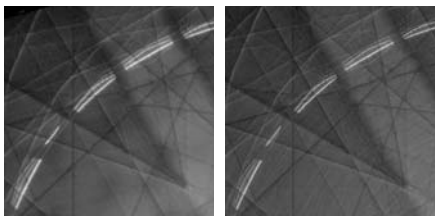
Si[111], 100kV, thickness 150nm

Calculation of TDS background (Kikuchi bands and lines)



experimental simulated

Left - experimental zero-loss energy filtered (20eV slit) CBED pattern of Si[111] at nominal 100kV. Image is courtesy by Prof. K.Tsuda.
Simulation of Si[111] for the best fit 100.9kV at 164nm thickness.
Intensity of both images is in log scale in order to reproduce both zero order disks and background.
Frozen phonons calculation in accordance to Einstein model (no correlation of atomic displacements) was used.
As it was already pointed out [C.R.Hall, Phil Mag 12 (1965) 815], [D.A. Muller et al., Ultramicroscopy 86 (2001) 371] Einstein model underestimates TDS in Bragg directions.



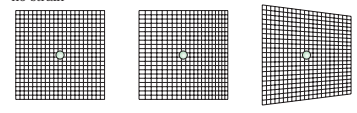
Enlarged sections of CBED patterns above. Fine structure of HOLZ and Kikuchi lines is perfectly reproduced in simulation. Integral intensity of HOLZ lines corresponds well for simulation and experiment (patterns intensity was normalise to central disk intensity), while TDS background is underestimated by about 20% (see also [R.F. LOANE, P. XU, J. SILCOX, Acta Cryst, A47 (1991) 267-278]). Experimental pattern looks more blurred because of finite width of the energy slit.

Calculation of CBED patterns for crystals with strain gradient

Si[331] at 100kV, thickness 237nm, no strain

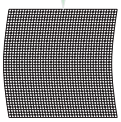
$\frac{\partial e_{xx}}{\partial x} = 4 \cdot 10^{-4}\, nm^{-1}$

$\frac{\partial e_{yy}}{\partial x} = 4 \cdot 10^{-4}\, nm^{-1}$



Si [230], 200 kV, thickness 300 nm

$\frac{\partial e_{xx}}{\partial z} = 1.5 \cdot 10^{-6}\, nm^{-1}$



A. Chuvilin, U. Kaiser,
Q. de Robillard, H.-J. Engelmann,
On the origin of HOLZ lines splitting near interfaces: multislice simulation of CBED patterns JEM, *in press*