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On the peculiarities of CBED pattern formation revealed by multislice simulation

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Abstract

A modified multislice method has been developed for calculations of Convergent Beam Electron Diffraction (CBED) patterns. The validity of the method for HOLZ- and Kikuchi-line calculations has been proofed by comparison to Bloch-wave calculations. The application of the method leads to the new understanding of CBED patterns formation. Dynamical scattering of weak HOLZ reflections plays the key role in the appearance of deficient lines in the central CBED disk. Different HOLZ lines do have significantly different and extended scattering areas; the central 000 CBED disk, consequently, contains structural information from an area around the primary beam which is determined by the Bragg angle of HOLZ reflections and the thickness of the sample. A variation of lattice parameters, if present within this area, results in artificial symmetry violations of the pattern and in changes of line profiles.

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1. Introduction

Convergent Beam Electron Diffraction (CBED) is a TEM technique with a wide range of unique capabilities. It can be applied for crystal symmetry determination [1], polarity determination of non-centrosymmetric crystals [2], temperature factors [3,4] and charge density refinement [5,6], dislocations and interface study [7–9], lattice parameter determination [10,11] and local strain analysis [12,13]. A few tasks, such as symmetry group or polarity determination, can be solved by direct interpretation of CBED patterns. However, for most of the tasks, especially if quantitative results are required, dynamical calculations of CBED patterns have to be performed, which are mainly based on the Bloch-wave approach [14,15] so far.

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Progress in semiconductor micro- and nanotechnology requires tools for the reliable local measurement of mechanical strains in semiconductor devices. The increasing popularity of the CBED method for this purpose is addressed to the thought that CBED patterns contain structural information from a column along the beam direction with a diameter of the area illuminated by the primary and strong diffracted beams [16]. Advances in field emission electron sources and electron optics made subnanometer size probes practically available, and thus strain fields in semiconductor devices might be measured with the spatial resolution of 1 nm. However, a number of phenomena have been observed in CBED patterns of imperfect crystals, which cannot be understood in the frame of this idea, as e.g. line splitting [17,18], unexpected symmetry violations [12] and HOLZ line blurring near the interfaces [19]. The Bloch wave theory cannot describe the scattering by imperfect crystals without further approximations, because of a huge number of Bloch states in this case and thus enormous computational expenses.

The multislice method was suggested as an alternative for calculating nanodiffraction [20]. Advantage of the multislice method is that it does not require particular approximations for imperfect crystals and thus electron scattering for the distorted crystals can be calculated to the same accuracy as for the perfect ones. Muller et al. [21] applied the multislice method to calculate correlated-phonon background in CBED patterns. Thus it was shown, that real-space information (correlation of displacements of atoms from outlying unit cells) is presented in experimental CBED patterns and can be reproduced using the multislice method. Also using the multislice method, Spence et al. [22,23] simulated successfully superstructural Laue rings from dislocation cores.

Here we demonstrate, that the multislice method can simulate correctly deficient HOLZ lines in the central CBED disk as well. Consequences of this approach seem to be of general value for the understanding of the process of CBED pattern formation and in particular to answer the question of how local a CBED pattern can be.

2. Methods

All simulations were performed with the homemade program "Mulsi" based on the implementation of FFT multislice algorithm. The algorithm was modified in accordance to Refs. [21,24] in order to optimise the speed of CBED calculations. "Mulsi" runs under Win2Kpro and higher on common use PCs. Depending on the hardware, the program allows at reasonable time (from a few hours to a few days on a P4 2.8 HT/2G RAM PC) the calculation of HR images and CBED patterns up to $8K \times 8K$ pixels in size of models consisting of up to 10^8 independent atoms.

The idea to calculate the propagation of a sharp electron probe with the multislice method was first introduced by Spence [20] and was utilized later for CBED [25] as well as for ADF STEM image calculations [26]. A focused probe is represented by a disk in reciprocal space (corresponding to electron wave filling the condenser aperture), rather than a delta function (plane wave) used for CTEM image simulations. The diameter of the disk determines the convergence angle of illuminating beam and the disk position determines the beam tilt. The modulation of the phase of the complex wave function within the disk allows accounting for lens aberrations and probe position in real space. The probe wave function in the real space is then obtained by a backward Fourier transformation.

Particular requirements for the calculation parameters have to be fulfilled in order to calculate CBED patterns including HOLZ lines. The sampling frequency in real space is determined by the scattering angle of the highest order lines included in the simulation. In order to account for the reflection with a particular g-vector of $G\,nm^{-1}$, the sampling interval of the phase grating should be smaller than $1/(2\,G)$ nm. For typical g-vectors of HOLZ lines of about $50\,nm^{-1}$, a sampling of at least 0.01 nm is required (which is similar to the requirements for HRTEM image calculations). The sampling interval in reciprocal space is determined by a desired resolution of HOLZ lines. In order to image a first-order Laue zone line (which is typically about $0.05\,nm^{-1}$ wide) with a width of at least two pixels, the sampling interval