Special aspects on the scattering of high-energetic electrons on crystals

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Quantitative analysis becomes more and more important in High-Resolution-Transmission-Electron-Microscopy (HRTEM). The current task of HRTEM-development is expanding the method from the sole characterization of the periodic structure to the determination of position and species of atoms within the specimen. Electron Holography is a unique technique capable of recording a 2-dimensional electron wave. In order to interpret this electron wave quantitatively, it is crucial to understand the interaction process between electron and specimen. Several methods have been developed to describe the scattering process. They offer a good qualitative description, although quantitatively they suffer from inaccuracy, which may contribute to the Stobbs-factor [1]. The problem has not been solved yet, although several proposals have been made.

In this work, some of those proposals have been compared analytically and quantitatively: The influence of the backscattered electrons, the singular structure of the scattering potential, and the thermal movement of the atoms within the solid. Firstly, the influence of the backscattered electrons is examined through the general solution of the stationary Schrödinger-Equation of a crystal as proposed by Lamla [2]. The only restrictions within that approach are posed to the geometry of the 3-dimensional crystal: The crystal is infinite in the directions perpendicular to the optical axis and finite along the optical axis. Within this geometry, the wave-function can be found by using a plane-wave-expansion in the vacuum region and a general Bloch-wave-expansion with complex Bloch-vectors in the crystal region. The solution does not incorporate approximations. The result raises questions with respect to the correct incorporation of the boundary conditions and hence the influence of the backscattered electrons, which are usually neglected. Secondly, the multislice method [3] is utilized to analyze the singular structure of the scattering potential. It is shown that screened atomic potentials with and without singularity produce a different behaviour in the simulation, especially at high sampling rates. The results are additionally compared with experimental data. Thirdly, concerning the thermal movement of the atoms it is shown that in electron holography an averaged 2-dimensional wave is measured and that the attenuation of the reflexions in Fourier-Space is not fully described by using the Debye-Waller-approach [4] originally developed for X-ray scattering.

It is demonstrated that all these factors produce effects, which might be not fully understood until now. This suggests that they probably contribute to the Stobbs-factor. Further investigations and developments are needed for a more appropriate consideration in image simulations.

References:

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