Quantitative Techniques and Image Simulation in TEM/STEM, SEM and Diffraction

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Influence of the delocalization of inner-shell excitations on atomic-resolution elemental maps

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In an aberration corrected scanning transmission electron microscope (STEM) the elemental distribution in a specimen can be investigated with atomic resolution using energy dispersive x-ray spectroscopy (EDX). For a better interpretation of the experimental results it is necessary to compare them with calculations in order to distinguish specimen properties from imaging artifacts. We investigate the influence of channelling and of the delocalized excitation of inner-shell electrons on elemental maps.

The behaviour of electrons passing through the specimen is described using the multislice method [1]. The intensity of characteristic x-ray quanta of an EDX experiment is proportional to the electron beam intensity near the respective specimen atoms. In a first approximation the atoms are approximated as being point-shaped. This corresponds to an extremely localized excitation which can be described by a δ-distribution. To improve this localized approximation we consider the atoms' excitation probabilities and replace the δ-distribution with a delocalized excitation function [2].

We compare the results of both approximations with each other and with experimental results to estimate the influence of an atom excitation probability on elemental maps.

Two samples serve as examples of our calculations: An interface between a zinc crystal and a bismuth crystal and an interface between a zinc crystal and a lead crystal. The first results of the simulation, calculated using the localized approximation, and the dark field image are shown in figure 1. For this calculation we assumed a sample thickness of 12 nm (10 slices), an acceleration voltage of 300 kV, a 34 mrad aperture semiangle, and an aberration corrected STEM.

The results show that the position of the boundary can be clearly discerned from the simulated STEM-image.

Currently we investigate how the elemental map changes when considering a delocalized excitation function in the simulation. These results will be compared with experimental data.

1. Earl J. Kirkland “Advanced Computing in Electron Microscopy” (Plenum Press, New York, 1998) p. 157
2. D. Von Hugo, H. Kohl, and H. Rose, Optik **79** (1988) p. 19

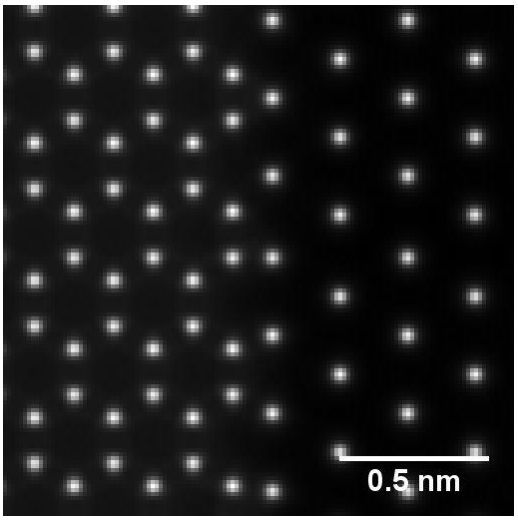

Figure 1. Simulated dark filed image of a Zn/Bi interface in [001]-orientation.

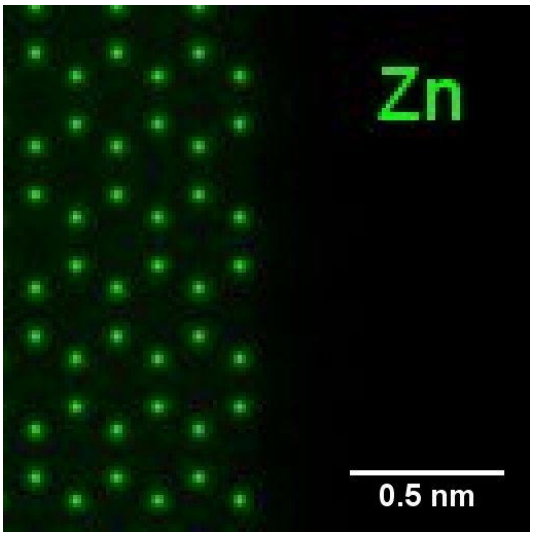

Figure 2. Simulation of the Zn-signal in an elemental map of 10 slices (≈12 nm) of a Zn/Bi interface simulated with localized approximation.

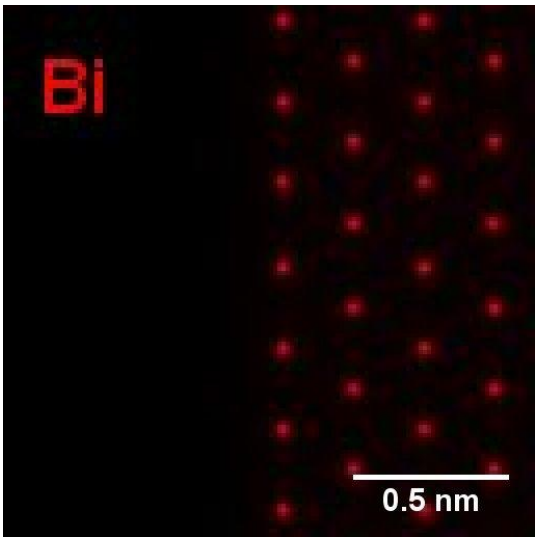

Figure 3. Simulation of the Bi-signal in an elemental map of 10 slices (≈12 nm) of a Zn/Bi interface simulated with localized approximation.