Quantitative High-Resolution TEM/STEM and Diffraction

IM.1.P016
Influence of the delocalization of inner-shell excitations on atomic-resolution elemental maps

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Keywords: STEM, EDX

Using energy dispersive x-ray spectroscopy (EDX) in a scanning transmission electron microscope (STEM) it is possible to obtain elemental maps with atomic resolution.

For a better interpretation of the experimental results it is necessary to compare them with simulations. The theory can show which factors influence the intensity distribution. In particular we investigate the influence of the delocalized excitation of inner-shell electrons on elemental maps using the multislice method [1].

The multislice method treats the behaviour of electrons passing through a thick specimen. For the simulation the specimen is divided into thin slices which are treated as a thin phase object. The transmission and the propagation of the electron wave function are calculated successively through and between the slices.

In a first approximation the intensity of characteristic x-ray quanta during an EDX experiment is proportional to the electron beam intensity at the respective specimen atoms. In this case the atoms can be approximated as being point-shaped. To improve this localized approximation we consider the atom excitation probabilities and replace the point-shaped description of atoms by a delocalized excitation function [2].

We want to compare the results of both approximations with each other and with experimental results to estimate the influence of the atoms' excitation probabilities on elemental maps.

For the simulation we assume a strontium titanate crystal ($SrTiO_3$). Figure 1 shows the structure of strontium titanate in different orientations. Figure 2 shows the simulation with the point approximation for the atom excitation probabilities of Sr-L and Ti-K signals in an elemental map of $SrTiO_3$ assuming an aberration corrected STEM using an acceleration voltage of 300kV, a spherical aberration coefficient of 0 mm, an aperture semiangle of 9.7 mrad, and a defocus of 0 Å. The size of the simulated image is 128x128 pixels [3].

These results are compared with experimental data. The major difference between both results is that the radius of the atomic columns is smaller in the simulation. This can be due to the point approximation for the atom excitation probabilities [3]. We want to investigate how the radius of atomic columns in the simulation changes considering a delocalized atom excitation function.

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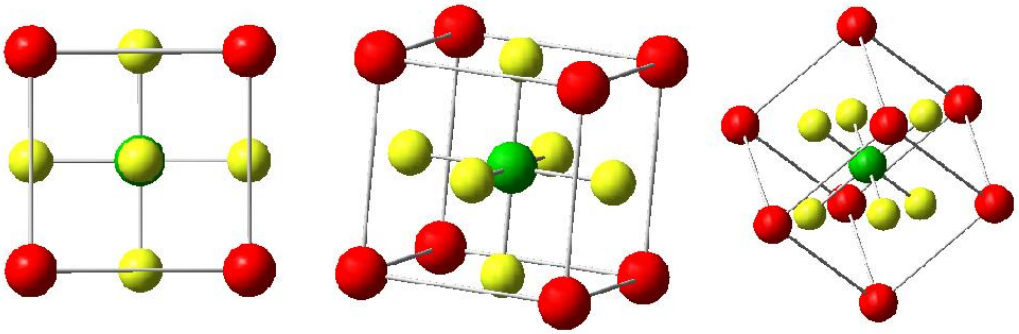

(a) (b) (c)

Figure 1. Structure of strontium titanate (red: strontium, green: titanium, yellow: oxygen); Simulations in the following figures conducted with a strontium titanate specimen in [001]-orientation (a).

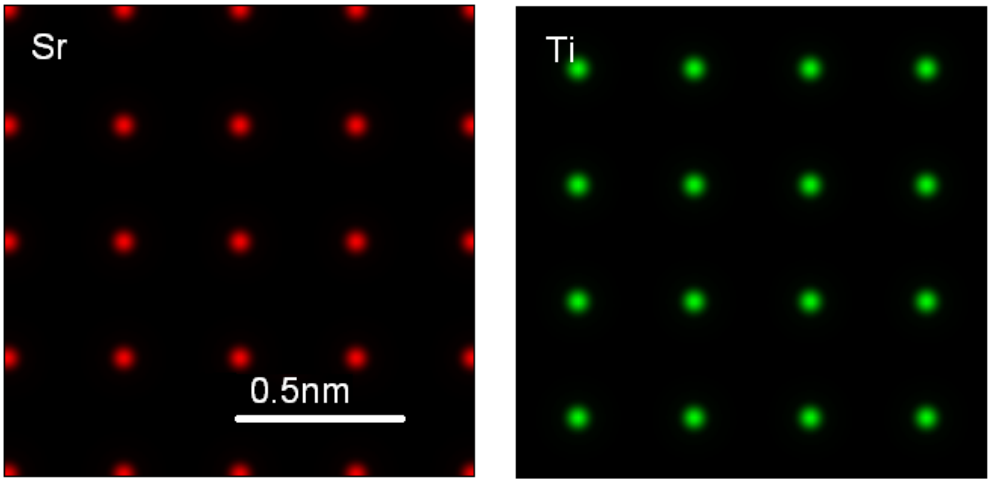

Figure 2. Simulation of Sr-L and Ti-K signals in elemental maps of $SrTiO_3$ assuming an aberration corrected STEM. The size of the simulated image is 128x128 pixels [3].