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IT-16-P-2768 Influence of the delocalization of inner-shell excitations on atomic-resolution elemental maps

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Using elemental maps with atomic resolution obtained by energy dispersive x-ray spectroscopy (EDX) in a scanning transmission electron microscopy (STEM), it is possible to investigate the elemental distribution in a specimen. To analyse the experimental results it is necessary to compare them with calculations in order to distiguish specimen properties from imaging artifacts. We investigate the influence of channeling and of the delocalized excitation of inner-shell electrons on the elemental map.

For our calculations, we use the multislice method [1], which describes the behaviour of electrons passing through a thick specimen. In this theorythe specimen is divided into thin slices treated as a pure phase object.

In a first approximation, we assume that the number of x-ray quanta emitted by an atom is proportional to the electron intensity at its position. This means that the atoms are approximated as being point-shaped. We then replace the point-shaped description of atoms with the delocalized excitation function [2].

To estimate the influence of an atom exicitation probability on elemental maps we also compare the results of both approximations with each other and these with experimental results.

An interface between a strontium titanate crystal ($SrTiO_3$) and a lead titanate crystal ($PbTiO_3$) serves as an example of our calculation.

The results of the simulation with the localized approximation of Ti, Sr and Pb signals in an elemental map of this sample are shown in Figure 1. For this calculation we used an acceleration voltage of 200 kV, assumed an objective lens free of astigmatism, a spherical aberration coefficient C_s = 0,5 mm, and a 15 mrad aperture semiangle [3]. These results are compared with the experimental data from L. J. Allen et al. [4].

The major difference between both results is that the position of the boundary is clear in the simulation but not in the experimental results. This could be the result of the unevenness of interface in the experiment and the use of the localized approximation in the calculation. For a better interpretation of the results we currently investigate how the radius of the atomic column and the boundary changes when considering a delocalized excitation function in the simulation.

[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

[3] S. Majert “Simulation atomar aufgelöster Elementverteilungsbilder mit der Multislice Methode”, BSc thesis (2012)

[4] L. J. Allen et al. “Chemical mapping at atomic resolution using energy-dispersive x-ray spectroscopy” (MRS BULLETIN, Volume 37, January 2012) p. 47

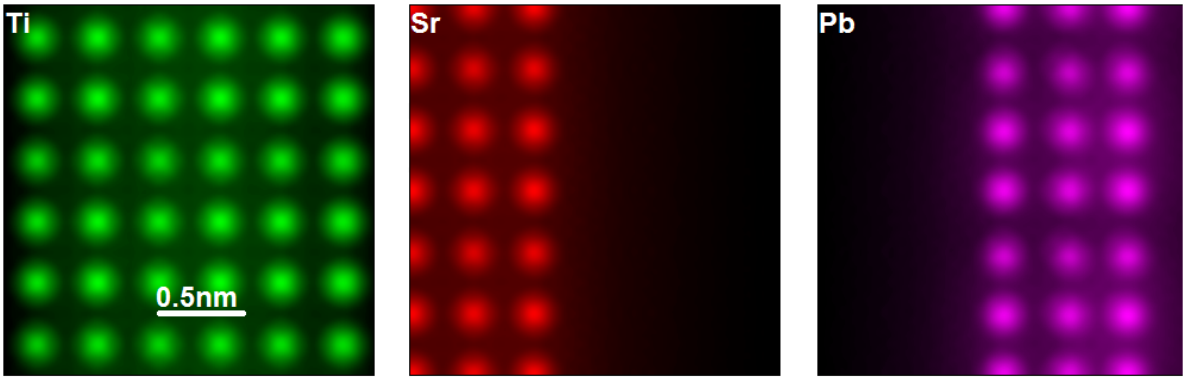

Fig. 1: Elemental map of 25 slices (≈10 nm) of an interface between a strontium titanate crystal ($SrTiO_3$) and a lead titanate crystal ($PbTiO_3$) in [001]-orientation simulated with the localized approximation