MS23. Nanoscale structures

Chairs: Joke Hadermann, Rainer Timm

MS23-O1 Crystallography using electrons: a focus on thin film materials

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Using strain engineering, metastable phases with original structures can be stabilized in the form of thin films. While X-ray diffraction is the most widely used technique to investigate the structure of materials, in case of a thin film grown on a substrate, the geometry of the sample and the small diffracting volume reduce the interest of this technique [1]. Not limited by the size of the probe or the small volume of matter, transmission electron microscopy (TEM) and scanning TEM (STEM) are able to provide structural informations at the nanometer scale using imaging, spectroscopic or diffraction methods. This will be illustrated with our recent analysis [2] of the $Bi_3Fe_2Mn_2O_{10+d}$ (BFMO) thin films [3] having a, previously unknown, layered structure formed by the alternative growth of Bi_2O_2 and $(Fe_{0.5}Mn_{0.5})_2O_4$ layers (see Figure). Using aberration-corrected STEM in high angle annular dark field (HAADF) and annular bright field (ABF) mode, prior crystallographic knowledge can be accessed by direct visualization of the structure with atomic resolution for both heavy and light elements. The ambiguous distribution of Fe and Mn cations within the $(Fe_{0.5}Mn_{0.5})_2O_4$ layers was resolved by high-resolution energy-dispersive X-ray spectroscopy mappings and, finally, the structure was solved using Precession Electron Diffraction Tomography (PEDT).

While challenging, the determination of unknown structures does actually not represent the major need for thin films. In most cases, the deposited materials have a known structure. The question is not to solve the structure but to know how it differs from the bulk. To this respect, electron microcopy has made enormous progresses towards quantitative and accurate structural analyses at nanoscale [4-5]. In the last part of this contribution, we would put an emphasis on the recent implementation [6] in JANA2006 of refinements based on the dynamical diffraction theory that opens the route for accurate structure refinements using electron diffraction data. Its application to the case of thin film materials will be discussed.

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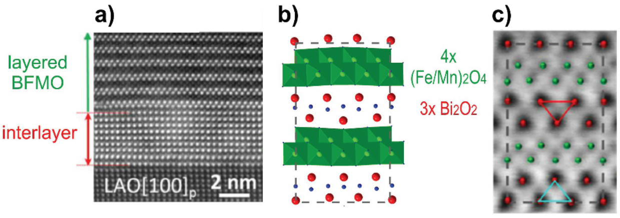

Figure 1. *a) $[100]_p$ STEM-HAADF image of a BFMO film, b) structure of layered BFMO obtained from PEDT (Bi: red, Fe/Mn: green, O: blue) and c) corresponding high-resolution STEM-ABF image taken along the $[010]_p$ zone axis.*

Keywords: electron crystallography, thin films, structure refinement