Sample Tilt Effects on Atom Column Position Determination in ABF-STEM Imaging

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The determination of atom positions from atomically resolved transmission electron micrographs is fundamental for the analysis of crystal defects and strain. Annular bright field (ABF) imaging in scanning transmission electron microscopy (STEM), has intrigued research interest in recent years due to its capability of direct visualisation of light elements, such as Li, N and O[1, 2]. The arrangement of light elements around heavy elements, such as the tilt of oxygen octahedra in complex oxides or the oxygen sub-lattice at complex-oxide hetero-interfaces, is accessible at the atomic-scale [3]. To extract reliable atom positions directly from the images one has to assume that the maxima/minima positions in ABF images precisely correspond to the atom positions.

In this work, we investigate the reliability of the atom column position determination in ABF-STEM imaging, with special emphasis on the influence of small specimen tilt from the zone axis. A glance of sample tilt effect on ABF/high-angle annular dark-field (HAADF) imaging is presented in Figure 1 which shows simulated results for cubic ZrO_2. Small specimen tilts can occur by inaccurate tilting by the operator, but can also have intrinsic reasons such as in the case of static tilts of crystal planes or atom columns near crystal defects. Quantitative interpretation of both experimental HAADF and ABF images with simulated results reveals the complex behaviour of the maxima/minima positions deviating from the expected positions in HAADF/ABF images when a small amount of local sample tilt exists. The reasons leading to these results will be discussed with respect to basic imaging theory. Suggestions on how to improve the precision on the determination of the atom positions in ABF imaging will be proposed. [4]

References:

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[2] S.D. Findlay et al, Appl Phys Lett, **95** (2009).
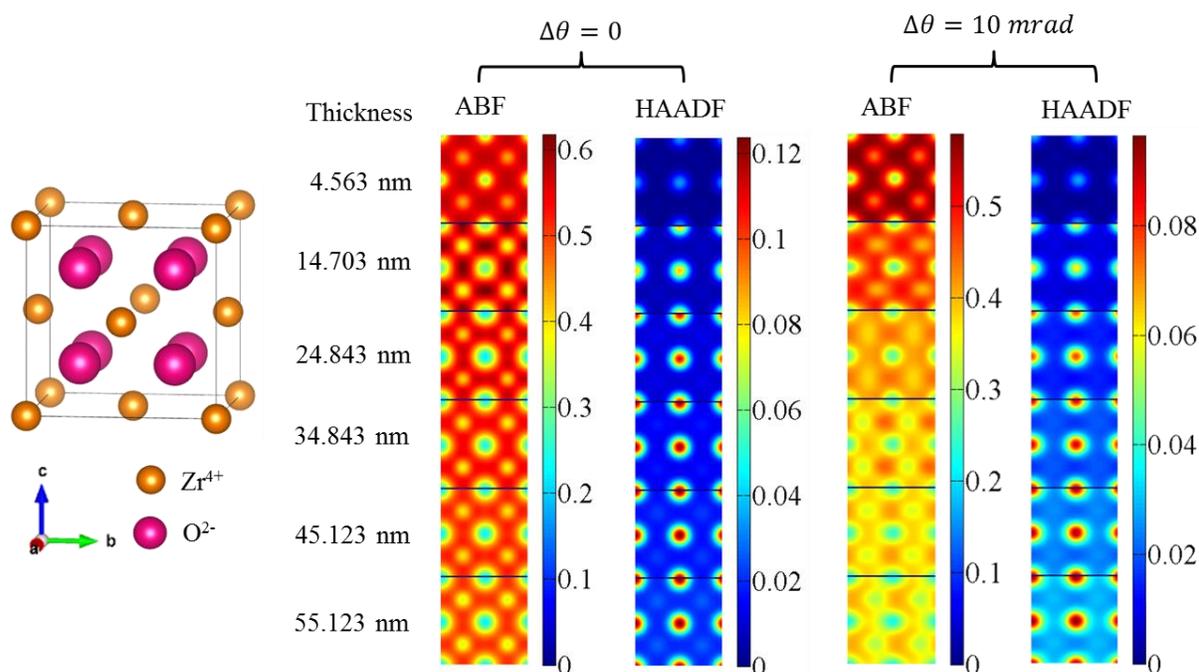[3] R. Huang et al, Adv Funct Mater, **24** (2014) 793-799.

Figure 1. Visualization of the effect of sample tilt, where $\Delta\theta$ is the amount of the sample tilt, on the variation of the minima / maxima position in simulated ABF/HAADF images of cubic ZrO_2 (see structure at the left) for different thicknesses. The central and right ABF/HAADF images are simulated for 0 and 10 mrad, respectively.