

Type of presentation: Oral

IT-2-O-1645 Atomically Resolved 3D Shape Determination of an MgO Crystal from a Single HRTEM Image

Jia C. L.^{1,2,3}, Mi S. B.^{1,4}, Barthel J.^{3,5}, Wang D.¹, Dunin-Borkowski R. E.^{2,3}, Urban K. W.^{2,3}, Thust A.^{2,3}

¹International Center of Dielectric Research, The School of Electronic and Information Engineering, Xi'an Jiaotong University, Xi'an 710049, China, ²Peter Grünberg Institute, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany, ³Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany, ⁴Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China, ⁵Central Facility for Electron Microscopy, RWTH Aachen University, Ahornstr. 55, 52074 Aachen, Germany.

Email of the presenting author: a.thust@fz-juelich.de

High-resolution transmission electron microscopy (HRTEM) allows one to investigate the structure of matter on an atomic level [1]. However, most atomic structure characterizations obtained by HRTEM were so far restricted to the determination of atomic column positions in the image plane perpendicular to the incident electron beam. Due to the fact that the depth resolution of the TEM technique along the beam direction is inferior to its lateral resolution, full 3D structure determinations on an atomic level remain highly challenging. The 3D structure retrieval problem can be solved with tomographic methods, where a multitude of images is acquired from different observation directions. Such multi-image approaches are very demanding at atomic resolution due to instrumental instabilities [2] and due to a possible radiation damage of the object. Alternatively, single-image approaches, where only one exposure is taken along a crystallographic zone axis, have been successfully used to count the number of atoms in crystalline columns running parallel to the beam direction. However, a full 3D determination of the crystal shape would additionally require a highly accurate determination of all column positions along the beam direction, which has not been achieved so far with the single-image approach.

We demonstrate that the full 3D shape of a thin MgO crystal can be determined in a nearly unique way from a single HRTEM image (Fig. 1). Our 3D determination of the crystal shape is based on refining an atomic structure model (Fig. 2) in such a way that a HRTEM image simulated on the basis of this model fits best to the experimental image. In contrast to the usual simplifying assumption of flat lower and upper object surfaces in conjunction with a single global defocus value [3], our structure refinement is executed now locally column-by-column, allowing also for atomically corrugated object surfaces. The comparison between simulation and experiment is made on the basis of absolute image intensity values [4]. A crucial part of our procedure is an extended statistical confidence test which yields detailed quantitative statements on the uniqueness and the reliability of the retrieved 3D crystal shape.

References:

- [1] K.W. Urban, *Science* **321** (2008) 506.
- [2] J. Barthel and A. Thust, *Ultramicroscopy* **134** (2013) 6.
- [3] C.-L. Jia et al, *Microsc. Microanal.* **19** (2013) 310.
- [4] A. Thust, *Phys. Rev. Lett.* **102** (2009) 220801.

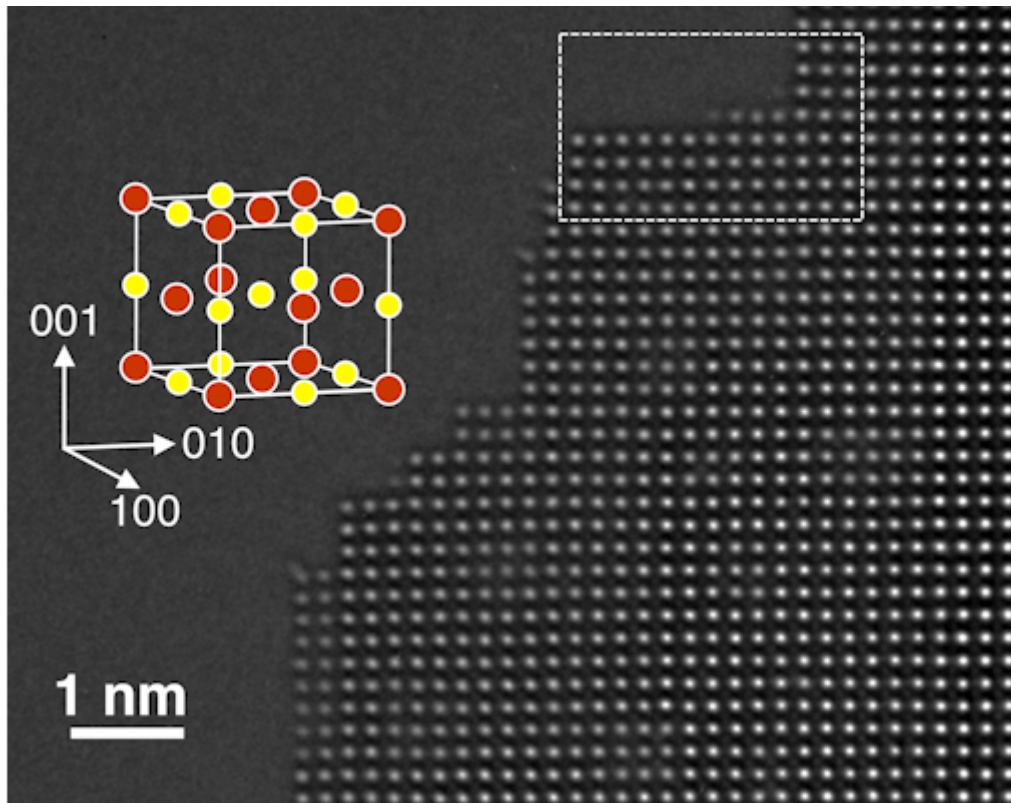


Fig. 1: High-resolution image of the edge of an MgO crystal taken along the [001] zone axis with a C_s -corrected FEI Titan 80-300 electron microscope at 300 kV accelerating voltage. The 3D shape reconstruction was performed at the area indicated by the dashed box.

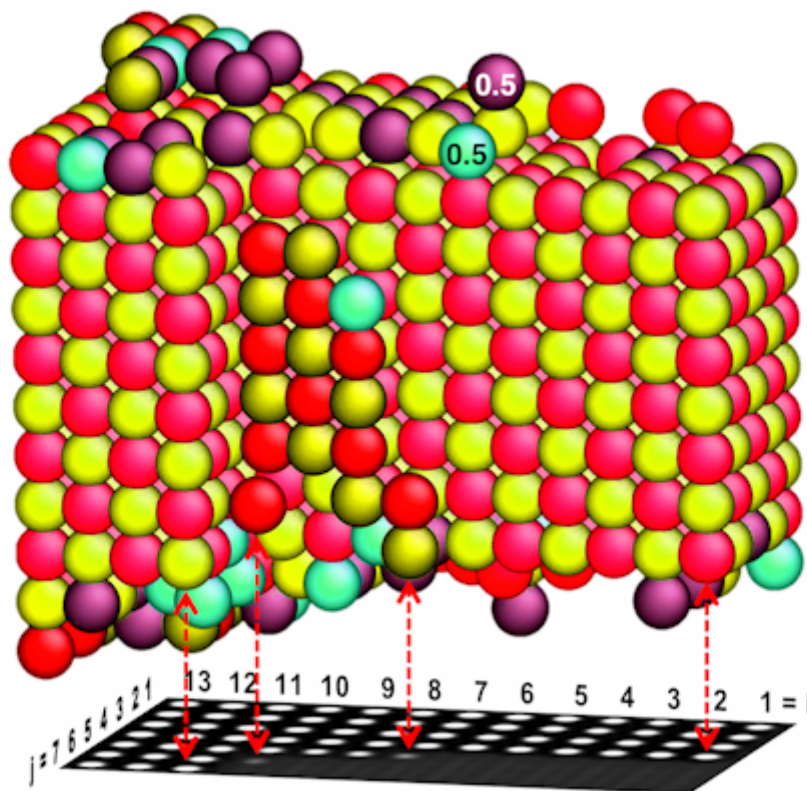


Fig. 2: 3D structure model retrieved from the boxed area in Fig. 1. Red balls indicate Mg atoms, yellow balls O atoms, purple balls indicate formally half-occupied Mg positions, and green balls formally half-occupied O positions.