DOI: 10.1017/S1431927603444668
Microsc Microanal 9(Suppl 2), 2003

HRTEM Imaging of Weakly Scattering Atom Columns Using a Negative Spherical Aberration Combined with an Overfocus

M. Lentzen, C.L. Jia, and K. Urban

Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

In modern high-resolution electron microscopy a careful alignment of the instrument removes aberrations, such as two-fold astigmatism, coma, and three-fold astigmatism. Then the image contrast is chiefly determined by the strong and fixed spherical aberration and the variable defocus of the objective lens. In recent years a prototype of a double-hexapole spherical-aberration correction system has been constructed by Haider et al. [1 3], following a suggestion by Rose [4]; it was adapted to a Philips CM200 FEG ST microscope with an information limit of better than 0.13 nm, installed at Jülich [5]. The aberration corrector allows an adjustment of the spherical aberration from the value of the uncorrected instrument over zero towards negative values.

The now variable spherical aberration C_S combined with the variable defocus Z provides new imaging modes [5]: $C_S = 0$ and $Z = 0$ leads to high-resolution amplitude imaging with vanishing delocalisation; a small positive C_S combined with a small underfocus extends the point resolution to the information limit, at a reduced level of delocalisation, producing a "black-atom" image of a thin specimen; a small negative C_S combined with a small overfocus extends the point resolution to the information limit as well, now producing a "white-atom" image of a thin specimen.

The white-atom imaging mode reveals experimentally a strong contrast modulation compared to the black-atom imaging mode [6]. A separation of the linear and non-linear contrast contributions to the image intensity shows: the reversal of the chief aberrations reverses the sign of the linear contributions, leaving their magnitude unchanged; the non-linear contributions do not change sign, reinforce the linear contrast in the white-atom case, and weaken it in the black-atom case.

The overall contrast improvement using a small negative spherical aberration combined with a small overfocus is in particular beneficial for the imaging of weakly scattering atom columns close to strongly scattering atom columns [6]. In an experimental study of $SrTiO_3$ [110] all types of atom columns could be resolved, in particular the oxygen sublattice (FIG. 1a). Because the information limit of our instrument is high enough to resolve the closest spacing between the oxygen and titanium columns, 0.138 nm, and the delocalisation is low, the image intensity provides local information on the scattering power of single columns. Comparing experimental intensity traces (FIG. 1b) with simulated intensity traces (FIG. 1c) provides now a simple means to measure the local oxygen occupancies, atom column by atom column. In another experimental study of $YBa_2Cu_3O_7$ all types of atom columns were resolved for the [100] and [010] zone axis, in particular the oxygen sublattice (FIG. 2). The image analysis of a stacking fault using both structure projections revealed a shift of one half of the [010] lattice parameter (FIG. 2a) and the occurrence of Cu-O double layer (FIG. 2b), indicating a so-called "124" fault. The enhanced white spot contrast of the Cu-O atom columns and the absence of contrast between these columns provides evidence for a highly perfect ordering, which can be explained by particularly strong Cu-O bonds along the [010] direction.

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[7] The project on aberration correction of a transmission electron microscope was funded by the Volkswagen Stiftung. The authors are grateful to Dr. Max Haider, CEOS GmbH, Heidelberg, for his kind and continuous support.

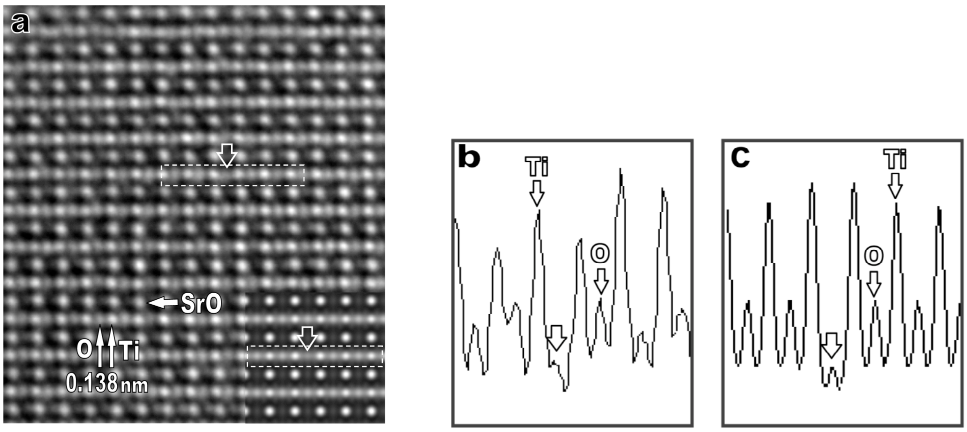

FIG. 1. (a) Experimental image of $SrTiO_3$ [110] at a specimen thickness of 4 nm, an overfocus of 8 nm, and a spherical aberration of □40 □m. The intensity of the oxygen column marked with an arrow is lower compared to other oxygen column positions. Inset: simulated image with an oxygen occupancy of 70% at one column. (b) Experimental intensity trace along the columns framed in (a): at one of the oxygen columns the intensity is reduced. (c) Simulated intensity trace with an oxygen occupancy of 70% at one column.

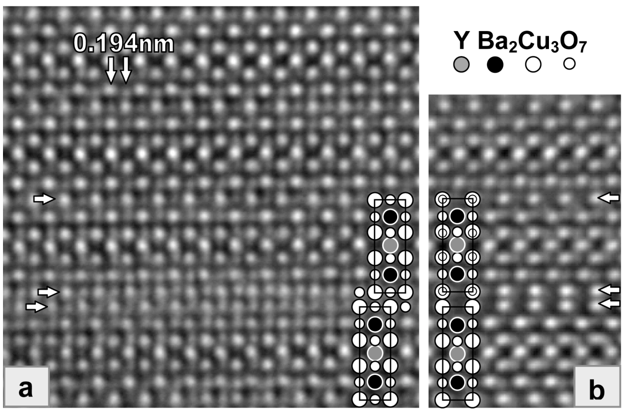

FIG. 2. Experimental images of a stacking fault, marked with double arrows, in $YBa_2Cu_3O_7$ at an overfocus of 12 nm and a spherical aberration of □40 □m. (a) Crystal in the [100] zone axis orientation. (b) Crystal in the [010] zone axis orientation.

https://doi.org/10.1017/S1431927603444668 Published online by Cambridge University Press