DOI: 10.1017/S143192760344467X
Microsc Microanal 9(Suppl 2), 2003
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Study of a ∑13 SrTiO3 grain boundary : Comparison between HREM, Exit Wave Reconstruction and Z-contrast analysis

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Electron exit wave reconstruction (EWR) has become a powerful tool to study defects and interfaces in solids [1-4]. Novel opportunities evolve with the application of this technique that can be complementary to other imaging techniques such as High Angle Annular Dark Field (HAADF) imaging or lattice imaging with high voltage microscopes. This paper addresses a comparison of the different imaging methods. A ∑13 grain boundary in a SrTi03 with a misorientation of 67°4 is used for this study. Classic HRTEM imaging was performed along [001] zone axis with a Jeol ARM operated at 800KV (point resolution :1.6 Å) , Electron exit waves were reconstructed from 20 lattice images recorded with a CM300 FEG/UT instrument (information limit : 0.8Å). HAADF images were obtained with a CM200 FEG/UT microscope (resolution :1.9Å). The HREM lattice image in figure 1 shows the periodic structure of the grain boundary. Details of the atomic structure will be found in reference [5]. Figures 2 and 3 show the same boundary recorded by EWR and HAADF imaging.

Differences between the recorded images are striking. In the lattice image shown in figure 1 strontium and titanium columns can be discriminated. In contrast, this is not the case in the reconstructed phase of the electron exit wave. In fact, image simulations show that the phase change on columns of Sr and Ti.O atoms are identical (figure 4). The rapid pattern change perpendicular to the boundary is caused by grooving of the sample along the grain boundary. Oxygen columns are readily visible. In the HAADF image Sr and Ti.O atom columns are clearly distinguishable but oxygen columns remain undetectable. In this respect EWR and HAADF imaging are truly complementary. In all cases, contrast changes occur close to the grain boundary that we attribute to the presence of grooving caused by the sample preparation technique. The origin of the contrast differences in images recorded by the mentioned techniques can be understood within the framework of theory[6].

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[6] The project was sponsored by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, and by French National National Center for scientific research and delegation generale de l'Armement under the contract No.ERE 03 60 034/DSP/SREA/SC/SR.

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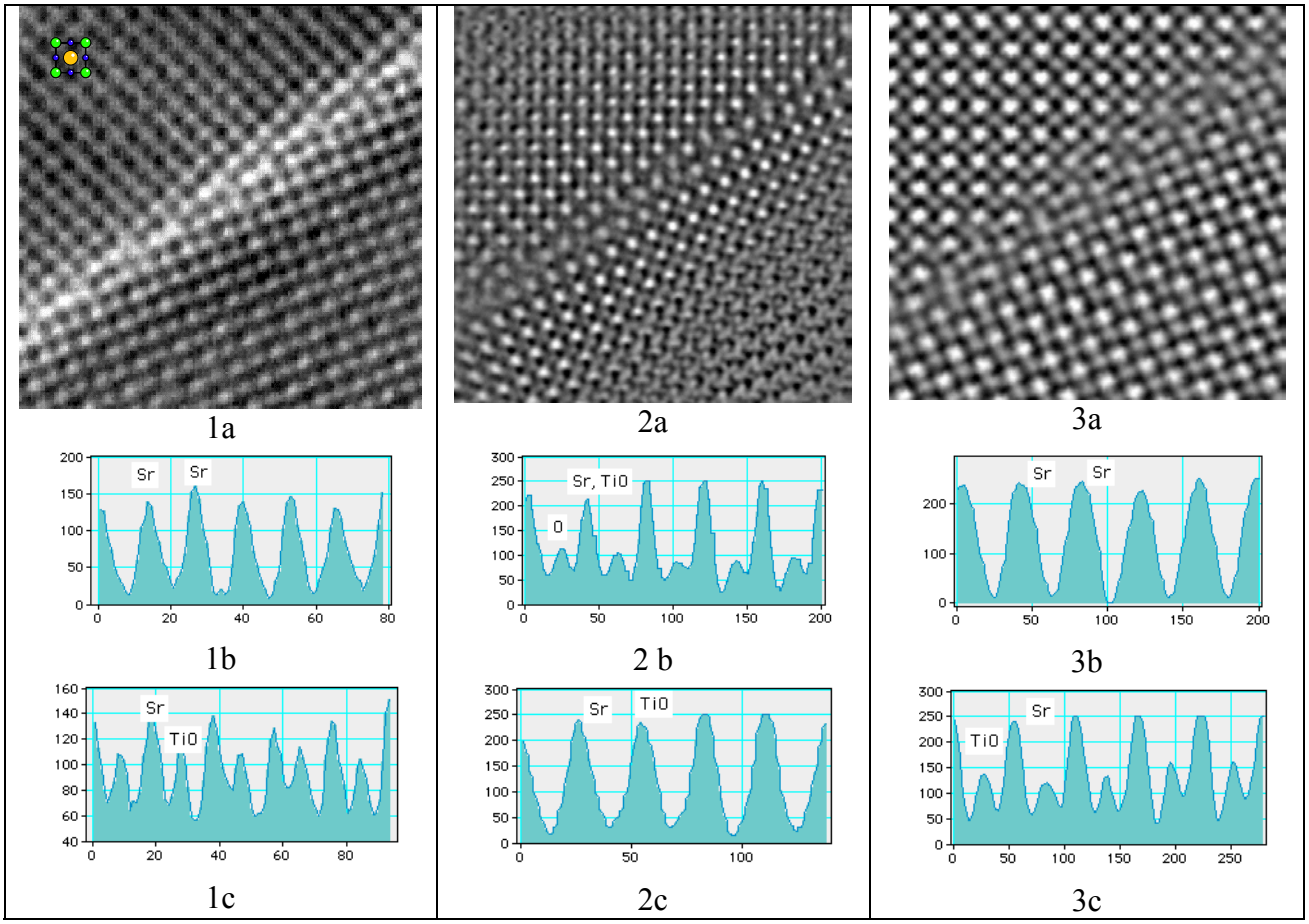
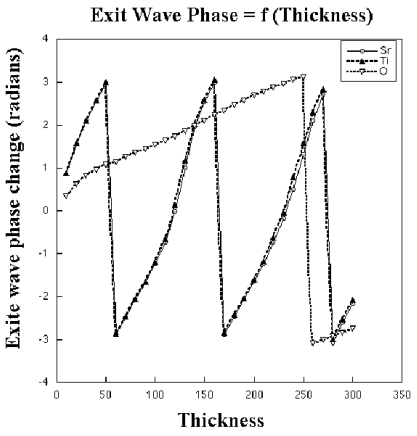
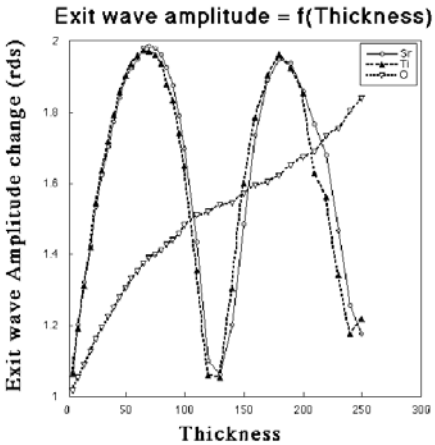


Figure 1 : Experimental HREM image (a) ; (b and c) Sr-Sr and TiO-Sr profiles.
Figure 2 : Experimental EWR phase image (a) ; (b and c) Sr-Sr and TiO-Sr profiles.
Figure 3 : Experimental Z-contrast image (a) ; (b and c) Sr-Sr and TiO-Sr profiles.



a



b

Figure 4 : (a) EW phase variation as a function of the thickness in Å; (b) EW amplitude variation as a function of the sample thickness in Å.