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To be presented at Microscopy and Microanalysis 2004, the annual meeting of the Microscopy Society of America, be held in Savannah, Georgia, August 1-5, 2004.

**High Resolution EELS with the Aberration Corrected STEM:
Determining Interfacial Electronic Structures with
High Accuracy**

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Prepared by the

CONDENSED MATTER SCIENCES DIVISION
OAK RIDGE NATIONAL LABORATORY
Managed by
UT-BATTELLE, LLC, for the
U.S. DEPARTMENT OF ENERGY
Under Contract DE-AC05-00OR22725

March 2004

High resolution EELS with the aberration corrected STEM: determining interfacial electronic structures with high accuracy

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Electron energy-loss near-edge structure (EELS) investigations have become an important technique for investigating bonding and electronic structures at homophase and heterophase interfaces. However, a very high spatial resolution along with a high energy resolution is crucial for obtaining highly localised electronic structure information.

So far, EELS investigations were performed as linescans across the apparent interfaces using electron probe sizes in the regime of 0.2nm. Energy resolutions in the regime between 0.5 and 1.0eV FWHM of the zero-loss peak were obtained, due to 3rd order aberrations of the electron spectrometer optics.

First results will be presented which were obtained with a third order aberration corrected parallel electron energy-loss spectrometer, which is attached to an aberration corrected VG HB501 UX dedicated scanning transmission electron microscope (STEM). This experimental setup consisting of a combination of the Gatan UHV Enfina spectrometer and the Nion Quadrupole Coupling Module [1] provides an energy resolution of better than 0.4eV FWHM of the zero-loss peak with spatial resolutions around 0.1nm.

Among other examples, we will report on the Pd/(100)SrTiO₃ interface, which shows a coherent and abrupt interface structure. Earlier investigations of this interface using the spatial difference technique indirectly revealed a TiO₂ termination of the substrate surface [2,3]. By comparison to *ab-initio* calculated unoccupied densities of states, the bonding behaviour at this interface was determined [3]. However, in this study we give direct evidence for the TiO₂ terminated interface structure in terms of high-angle annular dark-field (HAADF) imaging in the STEM (Figure 1a).

High-resolution ELNES data were recorded as linescans across the investigated interface using the aberration corrected Enfina spectrometer. Figure 2 shows the Ti L_{2,3}-edge and the O K-edge extracted from one linescan for three different positions: bulk SrTiO₃ (cyan), the terminating interface plane (red), and the Pd film (green). The crystal field splitting of the Ti edges is clearly resolved along with a slight reduction therein for the interface plane. The O K-edge, as smoothed by a 0.6 eV wide top-hat function is shown in the inset of Figure 2. Three interface peaks labelled X₁, X₂ and X₃ are observable, which are not present in bulk SrTiO₃. Calculated densities of states already predicted the presence of these peaks [3]. In contrast to X₃, peaks X₁ and X₂ could not be resolved during earlier studies [2,3] due to spectrometer aberrations limiting the experimental energy resolution. Correction of spectrometer aberrations coupled with spatial resolution at the Ångstrom level provides a new level of insight into interfacial structure-property relations.

[1] <http://www.nion.com>

[2] K. van Benthem, C. Elsässer, C. Scheu, W. Sigle, and M. Rühle, *Microscopy and Microanalysis 7*, Long Beach, Ca., USA (2001).

[3] K. van Benthem, doctoral thesis, U Stuttgart (2002):
<http://elib.uni-stuttgart.de/opus/volltexte/2002/1200/>

[4] The authors acknowledge fruitful discussions with O.L. Krivanek, A.R. Lupini, P.D. Nellist, M. Rühle, and C. Scheu.

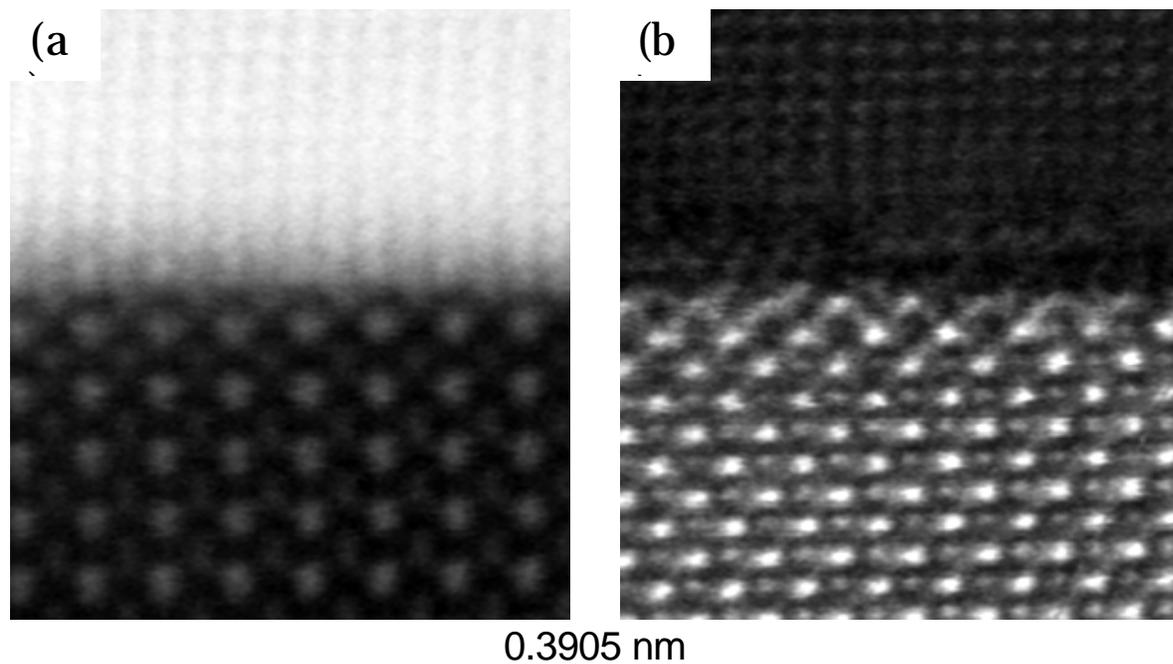


Figure 1: Annular dark-field (a) and incoherent bright field images (b) of the Pd/SrTiO₃ interface in <001> zone-axis orientation. Both images were acquired simultaneously with an aberration corrected VG HB603 STEM.

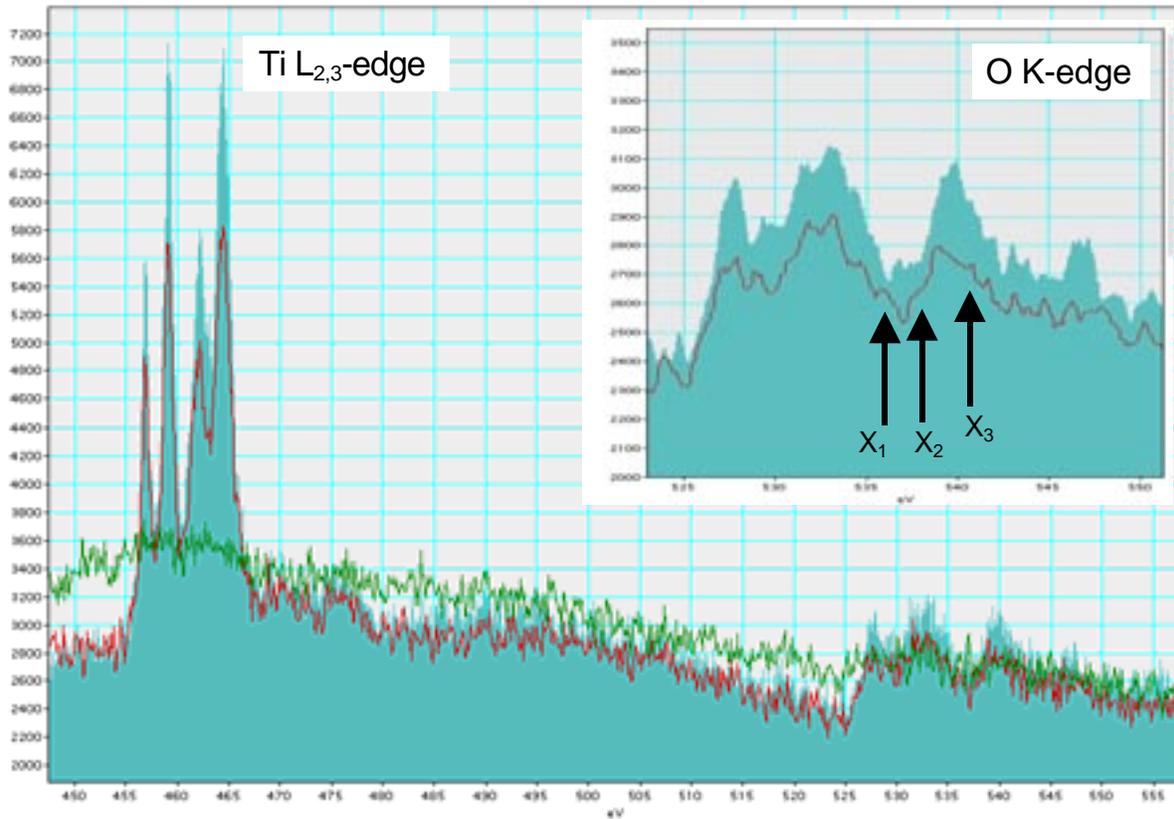


Figure 2: EELS spectra extracted from a linescan across the Pd/SrTiO₃ interface showing the Ti L_{2,3}-edge and the O K-edge. The O K-edge exhibits an interface peak in coincidence with calculated data and spatial difference results [2,3].