TOWARDS Z-CONTRAST IMAGING IN AN ABERRATION-CORRECTED STEM

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The demonstration of an aberration corrector for the STEM[1] promises enormous improvements in the contrast and signal to noise ratio of *Z*-contrast images, with similar benefits for atomic column EELS. Here we show that the limiting resolution for a zone axis crystal will become not the probe, as in the case of isolated atoms, but the 1s Bloch states. In fact, the *Z*-contrast image becomes a direct image of the 1s Bloch states with limiting intensities for large thicknesses roughly proportional to Z^2.[2] The potential benefits for the (STEM) appear to far exceed those for the conventional TEM. Some of these benefits are intrinsic to incoherent imaging: the lack of interference artifacts and the potential factor of two improvement in image resolution were first pointed out by Lord Rayleigh.[3] This improved resolution has been demonstrated by the achievement of sub-ångstrom information transfer in the VG Microscopes HB603U,[4] and the resolution advantage will still apply after aberration correction. In addition, for thickness independent structures, interpretation of incoherent images does not require accurate knowledge of defocus and thickness, nor extensive simulations of trial structures.

These benefits arise because of the large extent of the annular detector and central hole. The exact reciprocal space description of Nellist and Pennycook[5] allows the contributions of individual Bloch states to be determined, revealing the detected intensity to be dominated by the 1s Bloch states. The reason is that only highly localized states give a net intensity after integration over the large detector, less localized states destructively interfere. Now the image resolution is no longer the free space probe intensity profile, but an *effective* probe given by the convolution of the incident probe and the 1s Bloch state. Whereas today this causes only a slight broadening, as probe sizes are reduced through aberration correction, this effect will become more significant. Clearly, in the limit of a delta-function probe, we achieve a direct image of the 1s Bloch states themselves.[6]

The anticipated improvement in probe size is shown in Fig. 1. The FWHM intensity is predicted to decrease from the 1.3Å of today to only 0.5Å, with a significant increase in peak intensity assuming the same total current through the objective aperture. This will provide increased resolution, contrast, and signal to noise ratio. For example, the long-range tails of today's probe mean that it is impossible to detect light atoms close to high-*Z* columns. Figure 2a shows an image of a $SrTiO_3$ grain boundary in which the Sr and Ti columns are resolved and distinguished,[7] but the high background between the columns obscures the oxygen columns. In Fig. 2b the predicted 0.5Å free space probe is convoluted with a Z^2 delta function object , including estimated noise. The reduced range of the probe tails now allows the faint oxygen columns to be detected. In Fig. 2c the simulated image is convoluted with the 1s Bloch states which clearly degrades the resolution although the oxygen columns are still visible. Figure 3 shows an image of Pt atoms on crystalline γ-alumina obtained with the HB603U[8] with a simulated image using positions obtained from first principles density functional relaxations.[9] The simulation is for zone axis illumination using the free space probe for the Pt trimer layer and adding the simulation for ~5nm of substrate using the effective probe. The Pt atoms are still visible, smaller than the image of the Al and O columns of the support.[10]

References:

1. O. L. Krivanek, N. Delby and A. Lupini *Ultramicroscopy*, **78**(1999)1
2. B. Rafferty, S. J. Pennycook and P. D. Nellist, these proceedings
3. Lord Rayleigh, *Phil. Mag.* (5) **42**(1896)167
4. P. D. Nellist and S. J. Pennycook, *Phys. Rev. Lett.* **81**(1998)4156
5. P. D. Nellist and S. J. Pennycook, *Ultramicroscopy*, **78**(1998)111
6. S. J. Pennycook, B. Rafferty and P. D. Nellist, *Microscopy and Microanalysis*, in press
7. G. Duscher, N. D. Browning, and S. J. Pennycook, *Phys. Stat. Sol. (a)* **166**(1998)327
8. P. D. Nellist, and S. J. Pennycook, *Science* 274(1996)413
9. Karl Sohlberg, Stephen J. Pennycook, and Sokrates T. Pantelides, these proceedings
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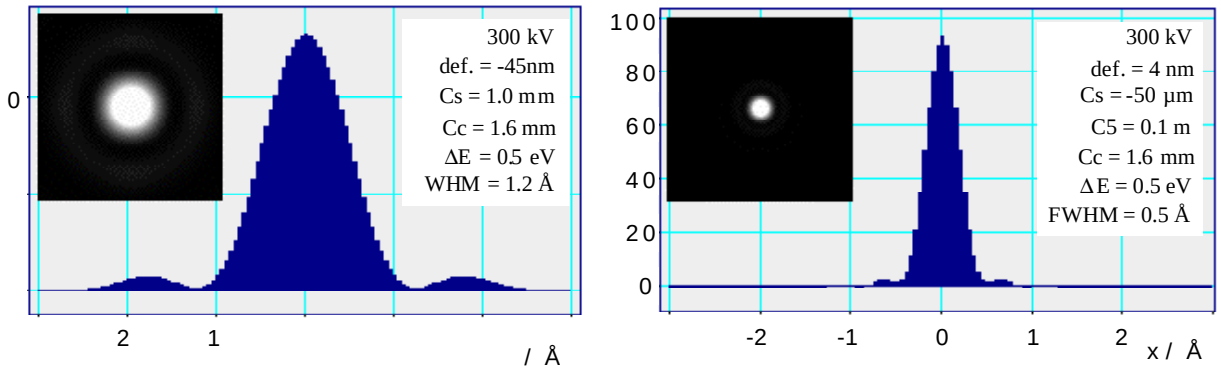

FIG. 1.— Theoretical probe profiles for the VG Microscopes HB603U STEM at ORNL. Left, today's probe with a 1.3Å FWHM, right, expected probe after correction of third order spherical aberration, showing approximately a 6-fold increase in peak intensity accompanied by a decrease in FWHM to 0.5Å and a reduction in probe tails (courtesy of O. Krivanek).

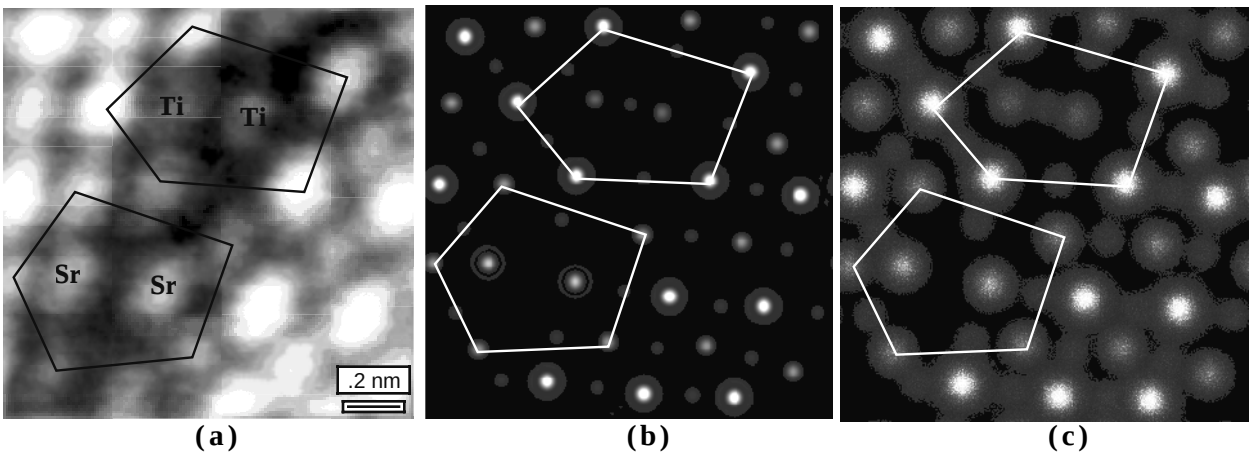

FIG. 2(a) Z-contrast image of a 36° $SrTiO_3$ grain boundary showing reconstructed Ti and Sr dislocation cores along the boundary plane. Simulated images for the aberration corrected STEM using the 0.5Å free space probe (b) and the effective probe after convolution with a 1s Bloch state (c).

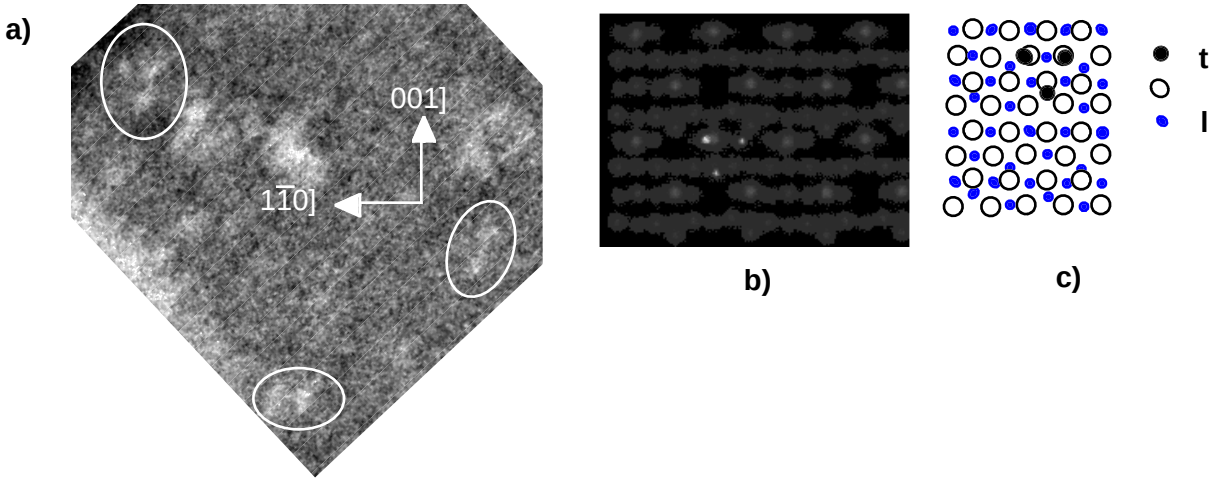

FIG. 3.— (a) Z-contrast image of Pt catalyst atom clusters ultradispersed on γ-alumina. (b) simulated image of a Pt_3 trimer for the aberration-corrected STEM. (c) relaxed structure projected along [110] showing Pt atoms occupying surface vacancies.