[Note: This is a reprint of an abstract. Contents of this document should not be quoted or referred to without permission of the author(s).]

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.

Tomographic Imaging of Nanostructures with Next Generation HAADF-STEM

Y. Peng, A. R. Lupini, A. Y. Borisevich, S. M. Travaglini, and S. J. Pennycook

Condensed Matter Sciences Division
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831

"The submitted manuscript has been authored by a contractor of the U.S. Government under contract No. DE-AC05-00OR22725. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes."

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

Tomographic Imaging of Nanostructures with Next Generation HAADF-STEM

Y. Peng, A. R. Lupini, A. Y. Borisevich, S. M. Travaglini and S. J. Pennycook

Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

Incoherent imaging by high angle annular dark field (HAADF) scanning transmission electron microscopy (STEM) has become a powerful characterization tool providing directly interpretable images of atomic columns at sub-Ångstrom resolution. Recently through Bloch wave calculations and multislice simulations, we have found a changeover from a projection mode of imaging to a depth slicing mode of imaging with increasing illumination angle. This new mode appears capable of resolving three-dimensional structures, even at the atomic scale in a future generation of aberration-corrected STEMs.

Bloch wave calculations [1] have shown that generally a HAADF-STEM image is a direct image of the 1s states for sub-Ångstrom probes as long as the 1s dominance is maintained. However, the non-1s component, which propagates essentially as plane waves, would give an increased contribution as the objective aperture is further increased, eventually destroying the 1s dominance. Consider the difference between Fig.1 (a) and (b) æ Due to the enhanced non-1s component at increased probe-forming aperture, the image function from a thin region will have significantly higher contrast with respect to the background than those from high thicknesses. This implies that, the image contrast and resolution at high thickness would be degraded due to the breakdown of the 1s dominance and channeling effect, while images at small thickness would remain with good contrast and even improved resolution. Since the non-1s component is scattered only weakly by the sample, it can thus come to a focus at a unique depth in the specimen. Therefore, experimentally if we defocus a "superprobe" so that it is brought to focus within the specimen, what the HAADF detector finally sees, due to the much reduced depth of field [2], would be mostly the image from that specific depth. Depth slicing and three-dimensional imaging may thus be realized as images are generated at different focal planes with next-generation Cs-corrected STEMs.

To justify the above inference, we calculated the contribution to the image from different depths within the specimen for an illumination angle of 35 mrad (probe size 0.29Å FWHM), with and without defocus. In the case without defocus (Fig. 2(a)), the first major valley lies at 28 Å and a small dip occurs at 8 Å, in good agreement with the analytical estimate and thickness-coherence prediction [1,3]. The difference between the peak contribution (at 5 Å) and any other region reaches a ratio of more than 3:1. With the introduction of a defocus of 50 Å (Fig. 2(b)), although the probe is less effectively focused inside the specimen compared with the no-defocus case, a steep peak remains in the region of 40 Å where the dumbbell structure can be distinctly resolved. The real image should thus be dominated by this characteristic depth. In further confirmation of this behavior, we present a multislice calculation in Fig. (3). By scanning the probe focused at different depths, we can simultaneously determine not only which atomic column the dopant atom is contained in, but also its depth within the specimen [4].

References:

[1] Y. Peng, P. D. Nellist, and S. J. Pennycook, *J. Electron Microsc.* (2004), in press.
[2] C. Dwyer and J. Etheridge, *Ultramicroscopy* **96** (2003) 343.
[3] D. E. Jesson and S. J. Pennycook, *Proc. Roy. Soc. London A* **441** (1993) 261.

[4] This work was supported by the USDOE under contract DE-AC05-00OR22725 managed by UT-Battelle, LLC.

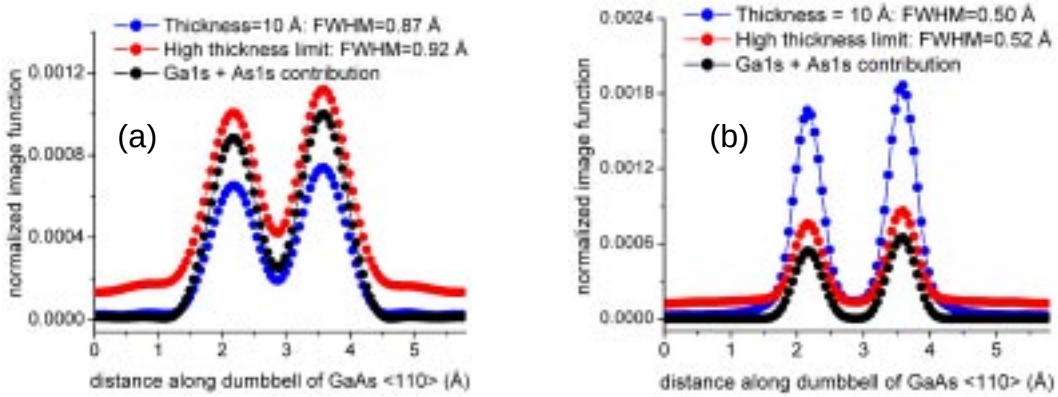

FIG. 1. Image function for small and high depths compared with the contribution from the 1s part, with (a) today's probe of 0.83Å FWHM, and (b) tomorrow's probe of

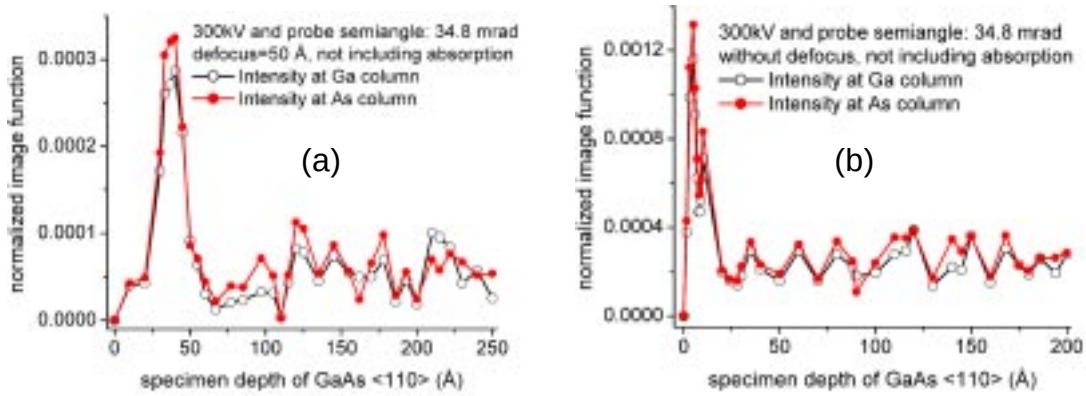

FIG. 2. Depth evolution of the image function in the case (a) without and (b) with defocus. This shows how much each depth within the sample contributes to the

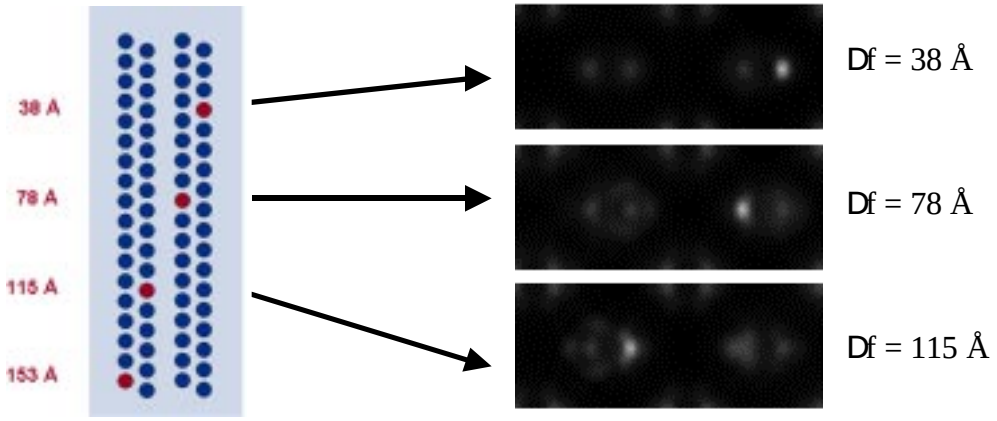

FIG. 3. Simulated HAADF images of Bi atoms embedded in a 160 Å thick Si crystal in the