

## Depth Sensitivity of Atomic Resolution Aberration-Corrected Through-Focus STEM Imaging of Bi Dopants on Cu Grain Boundaries

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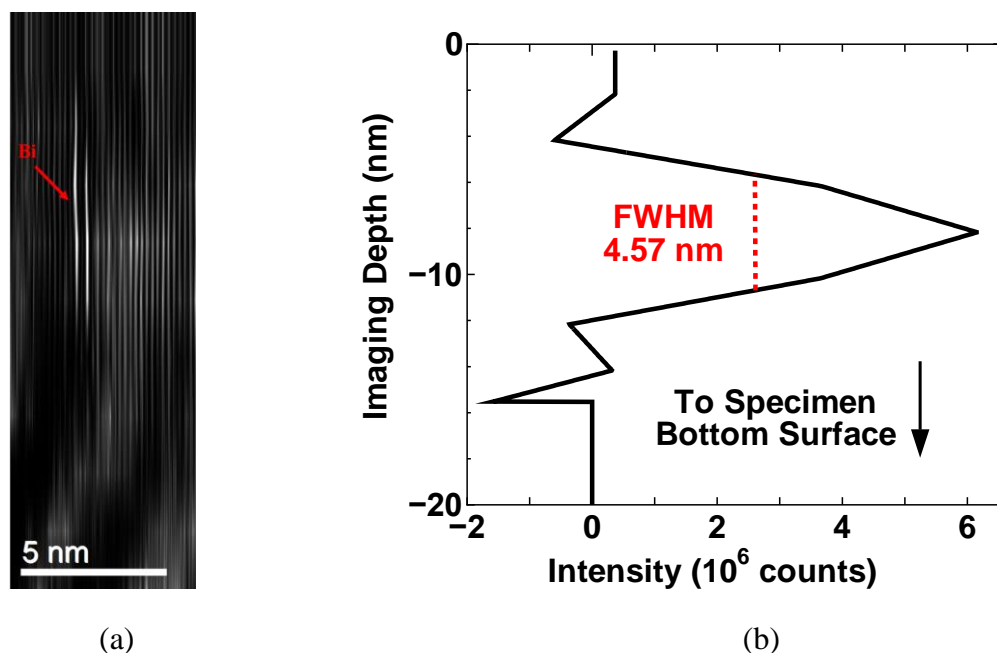
A complete 3-dimensional view of materials at an atomic level has long been a goal of modern electron microscopy. Difficulties in obtaining 3-dimensional images of materials at this high magnification level without the loss or distortion of information has been a challenge yet to be overcome [1]. The advent of an aberration-correction scanning transmission electron microscope (STEM) equipped with a cold field-emission electron source has allowed much higher beam convergence angles to be utilized without parasitic aberration degrading image quality [2]. The benefit of using a higher beam convergence angle is two-fold: first, the higher convergence angle offers an improved lateral resolution as lateral resolution is inversely proportional to the beam convergence semi-angle, and second, the vertical resolution (along the optic axis) is improved as the vertical resolution is inversely proportional to the square of the beam convergence semi-angle. With these benefits large convergence angles are increasingly being used for STEM imaging in aberration-corrected systems.

In this study the vertical resolution was measured by imaging single Bi atoms dispersed along a Cu bicrystal boundary as a function of the depth from the electron beam entrance (top surface) surface of the specimen. Of particular interest was how quickly vertical resolution would become degraded from various scattering events through the specimen and if through-focus STEM imaging was a practical approach to generating 3-dimensional images of these heavy dopant atoms along a grain boundary (GB). In the system studied Bi segregates almost exclusively to the Cu GB despite that the Bi atom location and the GB structure are not completely understood as it may change drastically depending on the geometric factors of the GB misorientation and the particular GB planes at GB of any given misorientation. By intentionally inclining the GB with respect to the incident electron beam, a specimen orientation in a near plane-view orientation is established, i.e. pseudo plan-view projection (PPP) imaging. From this orientation Bi atoms are laterally displaced from one another in the image projection that is formed allowing the image intensity of each Bi atom to be observed independently from any neighboring Bi atoms.

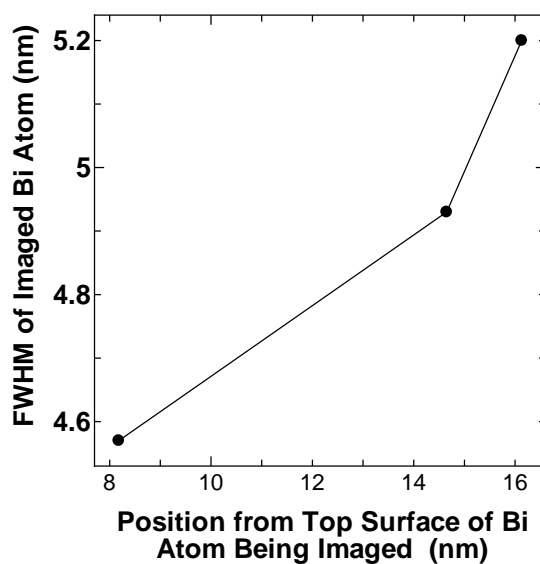
The best vertical resolution of a single Bi atom observed in this study was 4.57 nm. Figure 1a shows an x plane atomic number contrast (Z-contrast) image formed from a series of images obtained in a through-focus image series acquisition. The bright areas of this x plane Z-contrast image correspond to the high intensity generated from electron scattering off of the high atomic number Bi atoms. Figure 1b shows the intensity profile taken over one Bi atom, which represents the vertical resolution measured as the full width at half maximum (FWHM) value of intensity. Similar FWHM values may be measured from Bi atoms at several depths through the Cu specimen allowing the impact that the distance from the top surface of the specimen has on vertical resolution to be seen. Figure 2 plots the measured FWHM value of vertical Bi intensity as a function of the depth from the top surface. From this limited sampling it can be seen that the vertical resolution deteriorates rather quickly with increasing specimen thickness. These experimental results for vertical resolution were compared with simulated images of Bi atoms at various thicknesses in a Cu matrix.

## References:

- [1] H. L. Xin and D. A. Muller, *J Electron Microsc* **58** (2009), p. 157-165.  
 [2] A. R. Lupini *et al*, *Microsc Microanal* **15** (2009), p. 441-453.  
 [3] The authors acknowledge support NSF through grants DMR-0804528 and DMR-1040229



**Figure 1.** A Z-contrast intensity image (a) showing the vertical distribution of electron high-angle scattering from 2 Bi atoms on the Cu grain boundary in a PPP imaging orientation with (b) showing the vertical resolution, measured as 4.57 nm, given as the FWHM of intensity from one Bi atom in the Z-contrast intensity image.



**Figure 2.** A graph showing the decay of vertical resolution as measured Bi atoms were imaged further from the top surface of the Cu specimen.