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Limitations in Detecting a Single Dopant Atom Inside a Bulk Specimen

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3-D positions of single dopant atoms in a bulk specimen have been identified using scanning transmission electron microscopy (STEM) [1] and identity of dopant has been confirmed using electron energy loss spectroscopy (EELS) [2]. Many of these results have been reported on samples that were especially prepared for microscopy purposes. The techniques have yet to be standardized for routine work on unknown samples, but the successes so far and development of aberration corrected microscopes, reaching up to 0.5 Å probe size, and monochromators, limiting energy dispersion to 0.13 eV at 300 kV [3], promise a 3-D atom by atom reconstruction of hard materials in the near future.

In crystalline materials, electron channeling significantly changes the number of incident beam electrons along an atomic column parallel to the optic axis. As a result, depending on the position of a dopant atom, it may scatter many or few of the primary electrons. This, in turn, determines the visibility of a dopant atom. There are also many other factors that play a role in visibility of individual atoms.

Here, we have studied theoretically the limits of dopant atom visibility as a function of probe size, beam voltage, depth of dopant atom, specimen thickness, and the Z-difference between dopant element and bulk host. Visibility is defined as percent change in intensity between a doped and non-doped atomic column in an ADF-STEM image. We are interested in gauging the visibility of a single atom and what parameters must be adjusted to increase the visibility of an otherwise invisible substitutional point defect. Studies are based on multislice simulations [4]. In the figures shown here, parameters used to form aberration corrected STEM probe are: 100 keV incident beam, 25 mrad objective aperture, C_3 =-0.015 mm and C_5=10 mm spherical aberration coefficients, and -30 Å defocus, resulting in a probe size of 0.8 Å at FWHM. ADF detector angles used to collect scattered electrons range from 54º to 340º [5].

Results show that beam intensity profile along an atomic column does not correlate directly with changes in visibility of dopant atom due to its position along the column, implying that there are more factors affecting visibility than simply the number of electrons interacting with the dopant atom that come from the beam placed directly above it. For instance, type of the dopant atom plays a critical part, since changing the dopant element changes the trend in visibility (Figure 1). We observed that oscillations in visibility with depth of the dopant atom are not a function of specimen thickness (Figure 2). Visibility decays with increasing specimen thickness with a power law (Figure 3). We also observed that similar sized probes give similar visibility, regardless of voltage [6].

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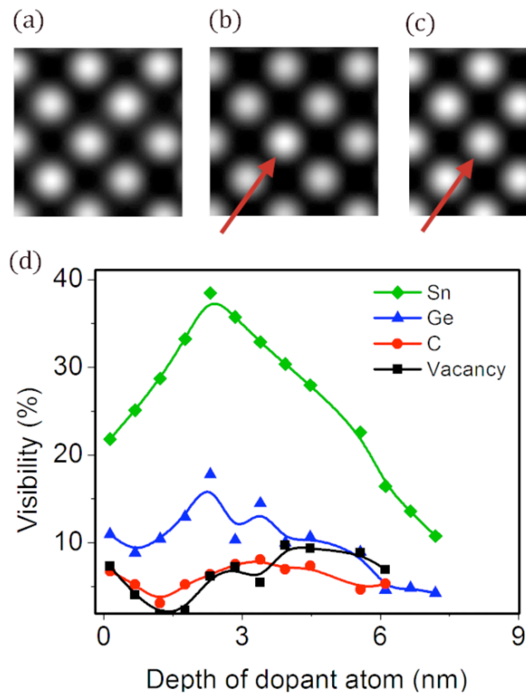

Figure 1

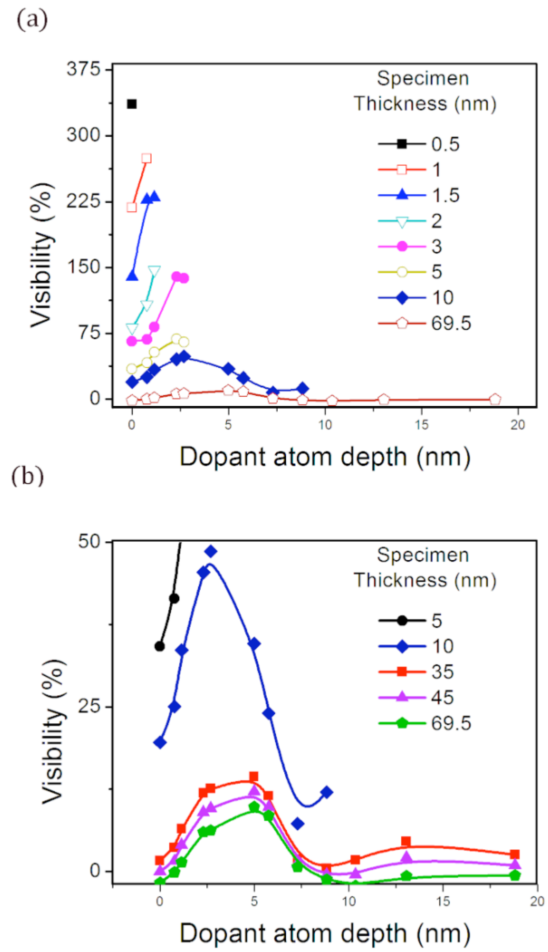

Figure 2

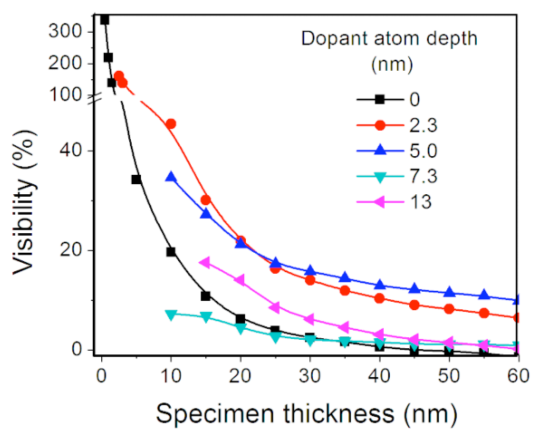

Figure 3

Figure 1. (a) Simulated ADF-STEM image of 25 nm thick Si oriented in 100 direction. (b) Surface doped with Sn atom and (c) with a vacancy point defect. Doped column is shown with a red arrow. (d) Visibility as a function of depth of dopant atom within the specimen.

Figure 2. (a) Visibility as a function of depth of dopant atom (Sn) in a Si specimen of varying thicknesses, oriented in 110 direction. (b) Vertical axis scale is changed to show the oscillations for thicker specimens.

Figure 3. Visibility as a function of specimen thickness for Si 110 specimen doped with Sn.

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