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Electron Channeling Artifacts in "Sub-Angstrom" STEM Images

Robert Hovden,* Huolin L. Xin** and David A. Muller*

* School of Applied and Engineering Physics, Cornell University, Ithaca, NY 14853
** Department of Physics, Cornell University, Ithaca, NY 14853

Aberration-corrected electron microscopes are now capable of forming deeply sub-angstrom probe sizes[1, 2]. Here we show that the standard resolution test of imaging a crystal along a zone-axis with closely spaced projected columns ("dumbbells") can fail dramatically at finite and realistic sample thicknesses due to electron channeling artifacts. This channeling can alter the image projected in a Scanning Tunneling Electron Microscope (STEM), changing the apparent resolution and perceived atomic positions. Most troubling of these artifacts is an apparent dumbbell shape that can still be present even when the initial probe lacks the information limit to detect the true spacing.

We report the effects of electron channeling in Si [211] through multi-slice simulation [3] (Fig 1). Simulated HAADF STEM images show shifts in the apparent atomic positions that depend on sample thickness and probe size. The shifts are opposite to those predicted from a simple incoherent imaging model where the initial probe shape is convolved with the projected-column object function. The incoherent imaging model predicts a decrease in perceived peak separation for sub-Rayleigh resolutions, described by O'Keefe as a "sub-Rayleigh shift"[4]. However, for all but the thinnest Si [211] samples, multi-slice simulations show a widening of peaks that significantly increases in the sub-Rayleigh regime due to extremely strong channeling of the probe wave function.

Simulations of Si [211] under sub-Rayleigh conditions have shown an apparent inter-column spacing increase to as much as 28% over the actual value of 0.78 Angstroms (Fig 2) – i.e, a dumbbell spacing is still present even when the initial probe is "larger" than 1 Angstrom. Such effects are clearly visible in Fig 1., which shows HAADF STEM images from multi-slice simulations of an aberration-corrected Titan (300 KeV). For aperture sizes below the incoherent Raleigh limit (fig1 a,d and b,e), false dumbbell spacings quickly develop in finite thickness (>5 nm) crystals. In addition, the increased inter-column spacing provides additional contrast of the two peak intensities and their central minimum and allows for increased apparent dumbbell resolution. This is seen in the 10mrad images: the 2nm thick sample only shows a single unresolved peak, while at 20nm two separate peaks appear. The result is apparently resolved dumbbells for apertures in the unresolvable sub-Rayleigh regime, where a dumbbell is defined as being resolved when the central minimum is greater than 26.5% below the dual maximum. This artifact can be checked by calibrating the image to the lower-order spacings in the image (e.g. {111}) and if care is taken to ensure a small enough pixel size and large signal/noise ratio.

For high resolution STEM it appears that tests of atomic-level performance will require calibration in order to pinpoint atom positions correctly and determine the resolution. By exploring electron channeling effects through theory and simulation, the effects on projected potential maxima can be characterized and used to estimate their actual positions [5].

References

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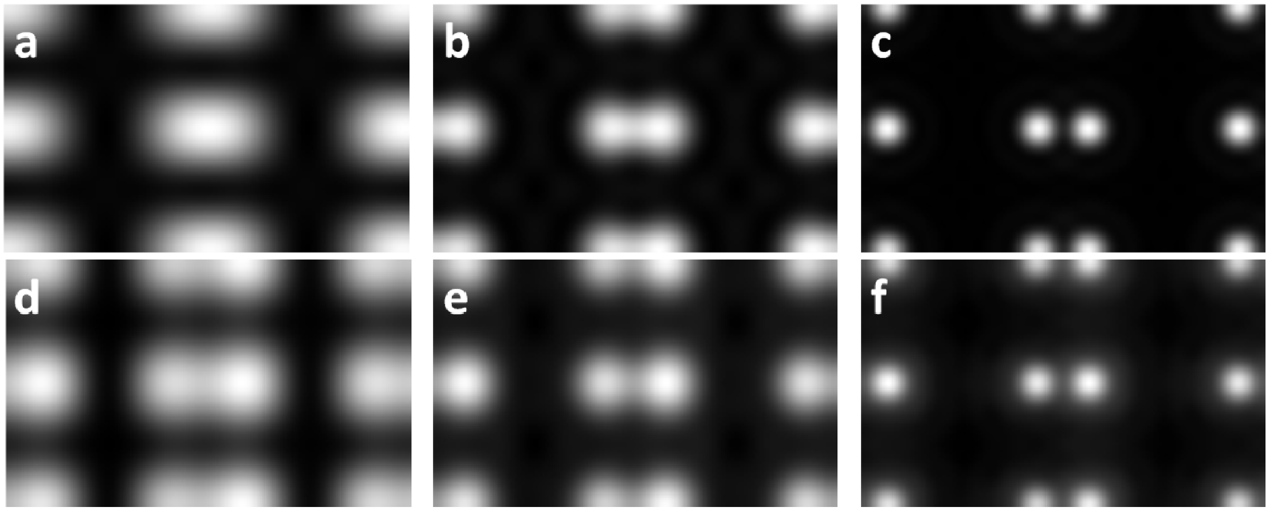

FIG. 1. HAADF-STEM multislice simulations of [211] silicon for a 300 KeV aberration-corrected instrument with probe-forming semi-angles of 10 (a,d),14 (b,e) and 23.8 (c,f) mrad and two different thicknesses, 2 nm (a,b,c) and 20 nm (d,e,f). For the 10 mrad aperture, the thin sample, a), is shown unresolved as a single peak but false dumbbells with two wider spaced peaks develop at more typical sample thicknesses, d). For larger apertures, as in (c,f), the effects are less pronounced.

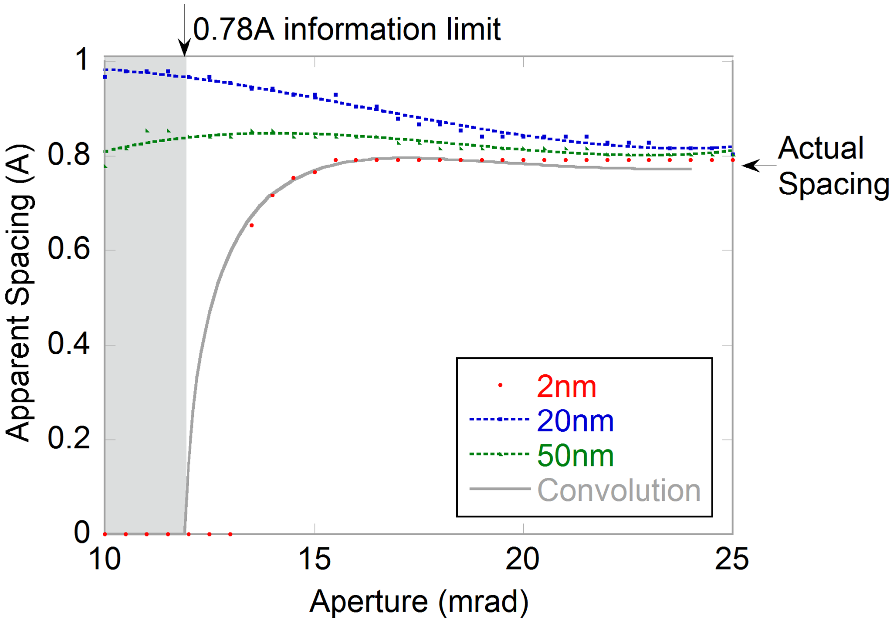

FIG. 2. Apparent separation of the [211] Si dumbbell for an aberration-corrected (C_5=20 mm) 300 keV Titan as a function of the probe-forming aperture size. Multislice simulations for 2, 20 and 50 nm thick samples are compared to the simple convolution of the ideal probe with the dumbbells. A false dumbbell with an incorrect spacing is present, even when the aperture is reduced below the information limit for the true dumbbell spacing.