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# Determining Resolution in an Aberration-Corrected Era: Why Your Probe is Larger Than You Thought

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Aberration-corrected electron microscopes are now capable of forming deeply sub-angstrom probe sizes. 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. Dumbbell features can be present when probe sizes are much larger than the inter-column spacing. In thicker samples these can be close to the correct spacing, but in thinner samples the spacing can appear wider than the actual distance. To show this experimentally, we imaged Si [211] with our aberration-corrected Nion STEM with a probe size larger than the 0.78 Å dumbbell spacing. Surprisingly, the peaks of two adjacent Si columns are present in the image, however, the spacing between them is measured to be ~1.4 Å, ~77 % larger than the actual spacing (Fig. 1). This raises the question of how resolution and probe size can be determined in the aberration corrected era.

To understand the deviations from the expected STEM images, a more complete understanding of fast electron propagation in crystals is needed. The propagation of swift electrons in materials can be complex and effects such as electron channeling (as seen in Fig. 2) have required full quantum mechanical multiple scattering multi-slice simulation for accurate analysis [1-3]. An approximation that has been used (perhaps implicitly) is essentially an independent-column approximation which assumes that the signal is focused and channeled down each column separately, as in Fig 2b.This is a reasonable approximation for large column spacings, such as when the microscope resolution was ~2 Å, but it fails dramatically when the column spacings become sub-Angstrom and transverse bound states from neighboring columns start to overlap (2c). Analogous to that of 2D hydrogenic atoms, the overlap of bound states gives rise to bonding and anti-bonding states. The maximum excitation of a dumbbell's anti-bonding state by an incident swift electron occurs on the outside of the inter-atomic positions of the two projected columns. The excited bound state then propagates and scatters resulting in an apparent increase in inter-atomic spacing of an incoherent elastic contrast image (Fig 1, Fig 3). As a consequence of the node in the anti-bonding state a double-peaked image occurs even for probes much larger than the true atomic spacings (Fig. 3) [4]. Only for atomically thin samples are these effects negligible and do the traditional resolution tests hold (Fig. 3). By treating the projected potentials of a crystal as 2D hydrogenic atoms, we are able to accurately model and greatly reduce the computational complexity of electron propagation in crystals (Fig 2d) The measurement of two peaks with an inter-peak spacing larger than the known atomic spacing, as shown in Fig. 1, is a direct result of probing the hydrogenic anti-symmetric bound state of the crystal. As a practical matter, dumbbell resolutions tests cannot be inferred from a single image, but need to be performed at series of well-determined thicknesses across the channeling regime.[6]

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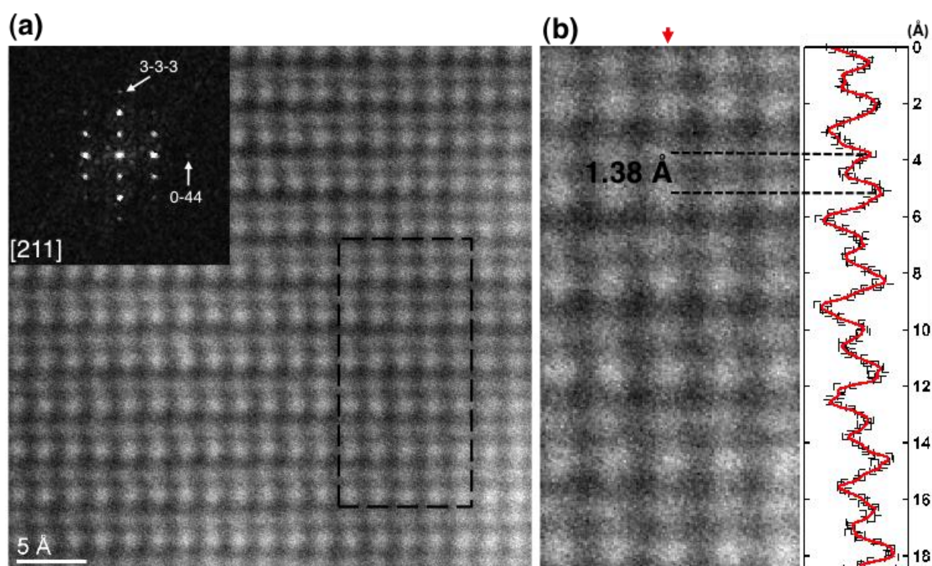


**FIG. 1.** An ADF-STEM image (cross correlation of 8 successively acquired images) of Si along the [211] zone axis acquired by a 100 KeV aberration-corrected Nion UltraSTEM (αmax = 33 mrad, I = 30 pA). Considering the resolution degradation from chromatic aberration and the incoherent source size, the 0.78 Å dumbbells are not expected to be resolved. However, the image still shows apparent [211] dumbbells, but their inter-column separation is ~77 % wider than the actual spacing.

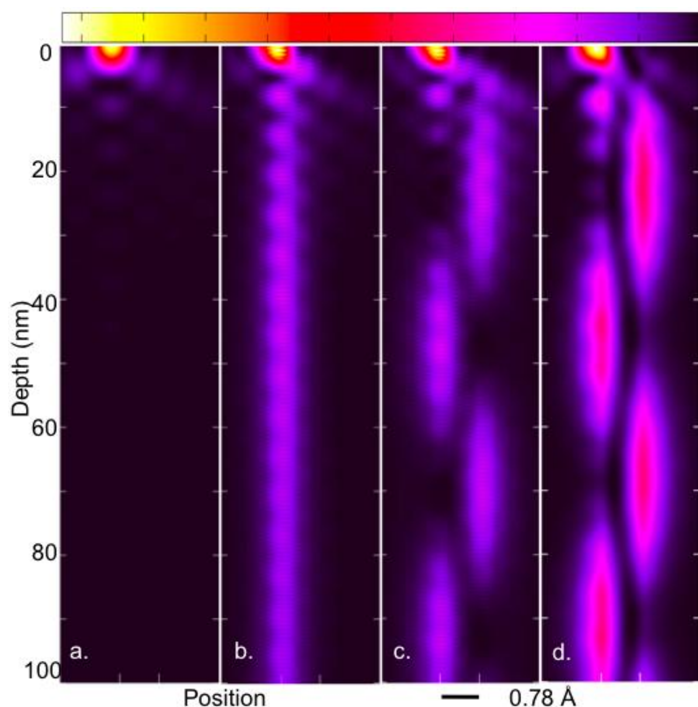


**FIG 2.** Cross sectional depth profile the of electron probe intensity (33mrad, 100keV) as it propagates down a) vacuum, b) a single Silicon atomic column and c) two adjacent columns simulated using multislice methods. d) The propagation of transverse eigenstates.

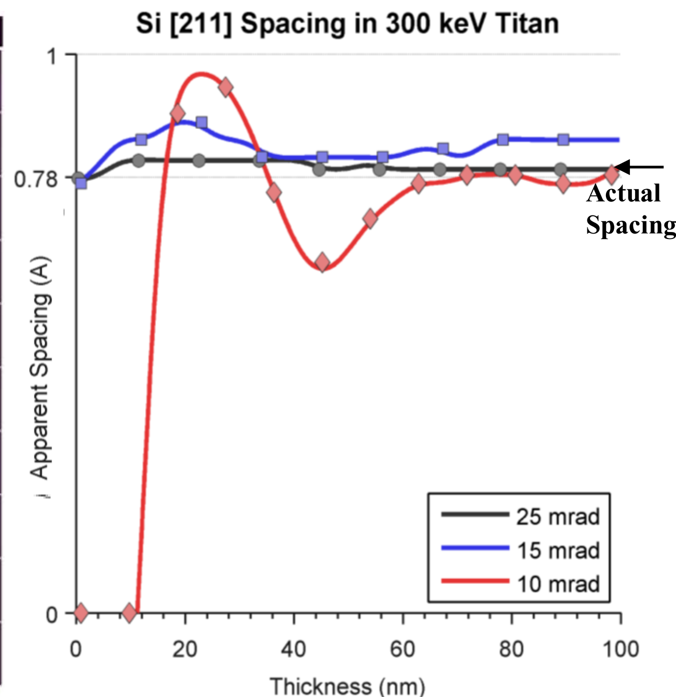


**FIG 3.** Simulated HAADF STEM Si [211] inter-column spacing as a function of sample thickness. For a typical TEM sample an dumbbell spacing is present, even when the aperture is reduced below the information limit (10mrad).

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