DOI: 10.1017/S143192760344470X
Microsc Microanal 9(Suppl 2), 2003

Ultimate Resolution Limit for ADF-STEM

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Recently of particular interest with scanning transmission electron microscope (STEM) is the pursuit of subangstrom resolution by use of spherical aberration corrector (for example, see Ref. [1]), which is motivated by the desire for single atom sensitivity in imaging and analysis, possibly even three-dimensional imaging of atomic structures. With the advance of state-of-the-art aberration correction, a new era is approaching in which the ultimate quantum mechanical resolution limit is to be reached, and theoretical attempt to address this issue is undoubtedly desirable.

Here we present some results from the Bloch wave approach [2,3], which has the strength of providing an insight into the physics of STEM image formation. Fig. 1 shows the image intensity profiles across the "dumbbell" structure for a thin and thick specimen of GaAs <110>. The intensity represents the coherent scattering reaching the detector from the respective thickness of the crystal. The effects of absorption and thermal diffuse scattering have been neglected in order to first understand the coherent scattering processes. The image shows clear peaks at the positions of the two dumbbell columns with 1.4 Å spacing, and the relative intensities show the expected atomic number, Z, contrast, with a distinct signal/background ratio of 4.5 ~ 6.5 even for the high thickness image. Comparison with the profile of the 1s Bloch states depicted in Fig. 2 shows that the image remains 1s-like at any thickness. Since one cannot expect to resolve structure below the size of a quantum state, the 1s state represents the quantum mechanical limit in a crystal. Resolution would be dominated by the size of the smallest 1s Bloch state or the STEM probe, whichever is less sharp. The full-width-half-maximum (FWHM) of the 1s states is around 0.3 Å, which is comparable to the size of the next generation probe after correction of aberrations up to 5^{th} order.

It is interesting that the ADF-STEM image persists to represent a direct image of the 1s states. An aberration corrected probe itself may have a very similar form to the 1s states. If a particle takes an eigenstates of a filter device, then it will be directly transmitted. Therefore, if the probe enters the crystal over an atomic column, it will match the 1s states and travel down the column, finally scattering to the ADF detector. This is the so-called channeling effect. If the probe is located between the atomic columns, since there is no 1s state to couple into, the probe will decompose into large number of less localized Bloch states which do not scatter efficiently into the detector. Furthermore, the probe will become narrower than a 1s state if the illumination angle is increased, and the coupling on the column will become less efficient. The illumination angle evolution of the overlap between the probe and the As 1s state is shown in Fig. 3 and a maximum appears at an angle of ~ 20 mrad. Beyond this angle, the contrast in the image, and possibly the image resolution itself, may decrease.

Fig. 4 shows the absorption-free thickness dependence of image intensity for GaAs <110> as calculated within the Bloch wave model. Although this is not representative of the physical image intensity that would be recorded in the presence of absorption and TDS, it does illustrate how interference between all the excited Bloch states leads to an extinction distance in the order of magnitude of 100 Å. The oscillation amplitude is seen to be about the intrinsic contrast contributed by the 1s states only.

References:

[1] P. E. Batson, N. Dellby and O. L. Krivanek, *Nature* **418**, 617(2002).
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[4] This work was supported by the USDOE under contract DE-AC05-00OR22725 managed by UT-Battelle, LLC.

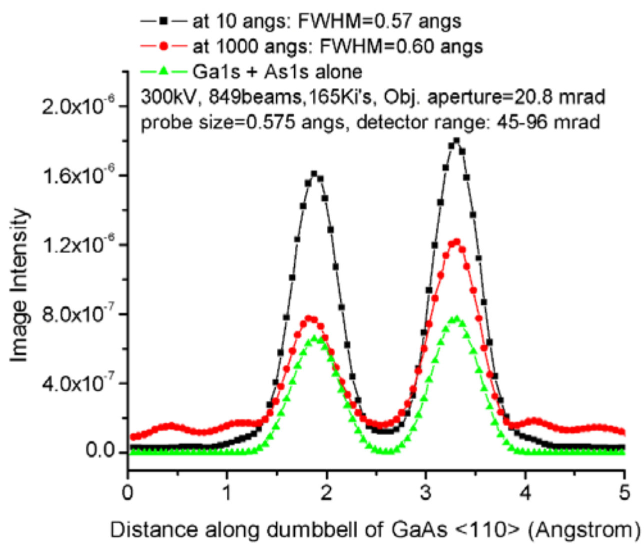

FIG. 1. Image profile for thin and thick specimen.

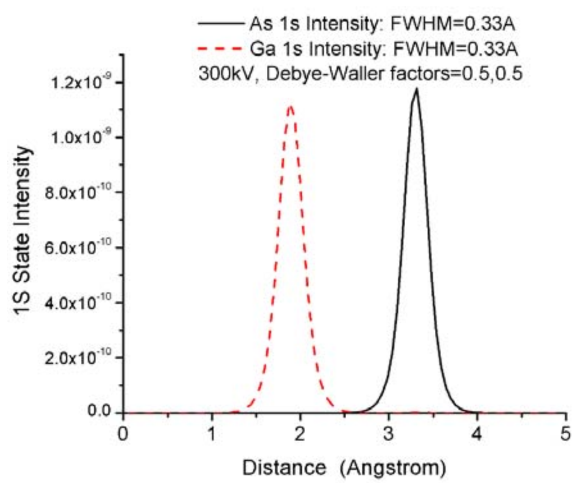

FIG.2. Intensities of 1s states in GaAs <110>.

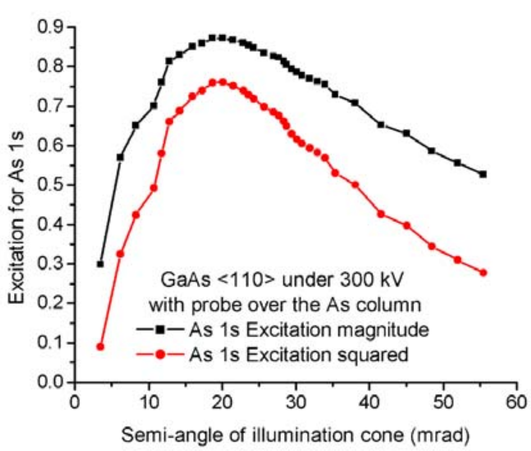

FIG. 3. 1s excitation vs. illumination angle.

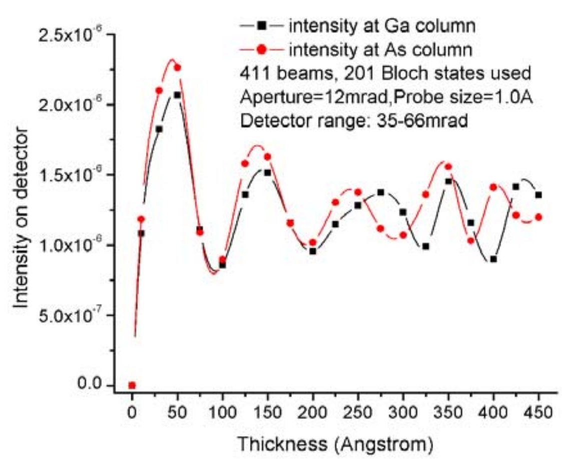

FIG. 4. Thickness dependence of ADF-STEM image.

https://doi.org/10.1017/S143192760344470X Published online by Cambridge University Press