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Annular dark-field (ADF) imaging in a scanning transmission electron microscope (STEM) at atomic resolution provides an incoherent image that can be described as the convolution between the intensity of the illuminating STEM probe and an object function consisting of localised sources at the atomic-column positions. It has been shown that the resolution limit of the microscope limits the accuracy to which the object function can be reconstructed [1]. Here we demonstrate how a number of images recorded at various degrees of underfocus can be reconstructed to give sub-ångstrom information, and discuss how quantitative physical measurements may be deduced from these images.

1. Sub-ångstrom imaging by underfocussing

The conventionally used optimum probe intensity profile for the VG Microscopes HB603U STEM (300 kV, C_S=1 mm), shown in Fig. 1a, requires an objective aperture radius of 9 mrad and 40 nm of underfocus. However, using a larger aperture and a greater degree of underfocus can give a probe with a much narrower central maximum (Fig 1b), but at the expense of creating side-lobes with increased intensity. Since this probe contains sharper features than the conventionally optimum probe, information at much higher spatial frequencies can be recorded. Figure 2 shows information transfer down to a resolution of 0.78 Å. Although the images recorded using such a probe are not as intuitively interpretable as those recorded using the optimum probe, the lack of a phase problem in incoherent imaging means that the probe may be immediately deconvolved from the image intensity data, and phase retrieval techniques are not required [1]. The geometry of ADF imaging makes this method robust to chromatic defocus spread, unlike focal-series reconstruction methods in conventional, coherent transmission electron microscopy.

2. Quantifying ADF STEM images

Two classes of information can be extracted by ADF imaging: The locations of the sources in the object function can be used to accurately measure the positions of the atomic columns to quantify the structure, and the intensities of the sources depend strongly upon the atomic number of the species present (Z-contrast) to reveal compositional information. Unambiguous determination of the structural information requires some form of prior knowledge, which can be incorporated using a Bayesian analysis [1]. Quantitative compositional determination requires some form of calculation (see for example Ref. [2]) that models the small residual coherence parallel to the electron beam. A Bloch wave approach shows that the object function is dominated by the tightly-bound 1s-type states (Fig. 3), which can be treated as being independent, incoherent scatterers with respect to their neighbours. Realisation of this opens the way for faster, simpler algorithms to calculate the expected column intensities.

References

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