

QUANTITATIVE INTERPRETATION AND INFORMATION LIMITS IN ANNULAR DARK-FIELD STEM IMAGES

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In making quantitative measurements using electron micrographs we must regard the electron microscope as being an information channel. The information about the object is both in some way transformed by the image forming process, and information is lost through the existence of a spatial resolution limit and the addition of noise. To make quantitative measurements, we need to take account of all these effects.

Great progress has been made in making quantitative measurements from high-resolution transmission electron microscope (HRTEM) images (for example see Ref. [1]). However, the simulation of HRTEM images requires a full dynamical electron scattering calculation in addition to computing the effects of the objective lens aberrations. Although such calculations can provide excellent agreement with experimental data, the calculation times involved restrict the number of trial structure models that can be used, with the danger that such trial and error methods might miss the true object solution. We aim for an imaging process that can allow direct inversion from the image to the object. Annular dark-field (ADF) imaging in the scanning transmission electron microscope (STEM) is an incoherent imaging mode that can be modelled as a simple convolution between the intensity of the illuminating STEM probe and an object function with localised peaks at the atomic column positions [2]. Here we only consider the positions of these peaks and the retrieval of structural information, though the strengths of the peaks can be used to retrieve compositional information [3].

Inversion from image data to an object function can therefore be achieved in principle by a simple deconvolution of the probe intensity from the experimental image. A problem arises, however, when atom columns are not resolved by the microscope (Fig. 1). Different deconvolution methods retrieve different object functions, all of which are consistent with the image, but none of which represent the original trial structure. This is a result of the resolution limit removing information during the imaging process, which means that the image cannot represent a unique object function. Constraints and prior information may be used to select a suitable object function, but it is always preferable to expand the amount of information transmitted by improving the resolution. Fig. 2 shows a simulated image using a highly underfocussed probe that has a complicated form and large side-lobes, but can pass higher resolution information. This time the CLEAN algorithm (see Ref. [2] for a description) provides an object function that is a good representation of the specimen, in spite of the complicated probe function.

An image taken using a VG Microscopes HB603U STEM (300 kV, $C_s=1$ mm) at large underfocus (-125 nm) does indeed show that information can be transferred through the microscope to resolutions better than 0.78 \AA (Fig. 3). It is somewhat surprising that the information transfer is not limited by chromatic aberrations to a worse resolution than this. The explanation is that chromatic aberrations affect incoherent imaging in a totally different way compared to HRTEM (Fig. 4) [4]. Rather than imposing a sharply truncated multiplicative envelope to the transfer function (as in HRTEM), chromatic aberrations lead to an upper limit to the transfer function: this upper limit being proportional to the reciprocal of spatial frequency. Although Fig. 3 contains a noisy image, the demonstrated robustness to chromatic aberration augers well for quantitative interpretation of incoherent images in spherical aberration corrected STEMs.

References

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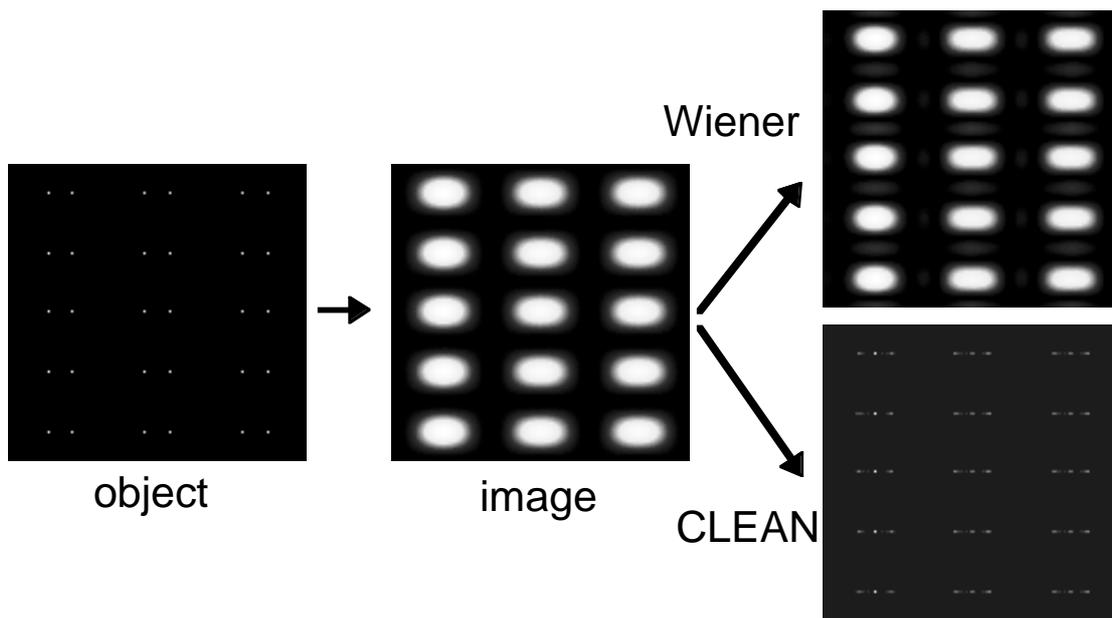


Fig. 1. A simulation of the imaging followed by probe deconvolution of Si<112> in the VG Microscopes HB603U at Scherzer focus. The column pairs separated by 0.13 Å are unresolved, and both a multiplicative (Wiener) deconvolution and the CLEAN algorithm reconstruct an object function unrepresentative of the specimen.

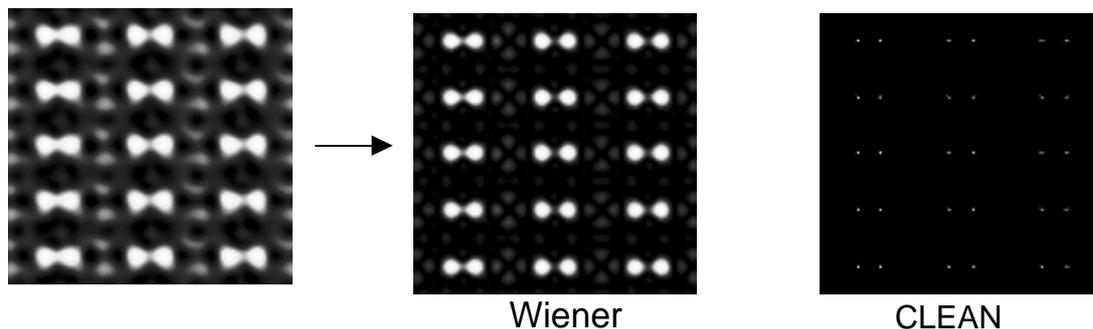


Fig. 2. A simulated image of Si<112> using a highly underfocussed lens (-125 nm). Although large side-lobe artefacts are produced, this time deconvolution methods are much more successful.

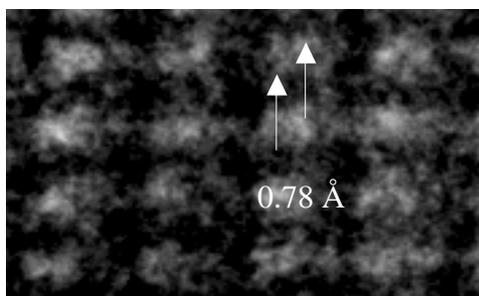


Fig. 3. An image of Si<112> taken at -125 nm defocus.

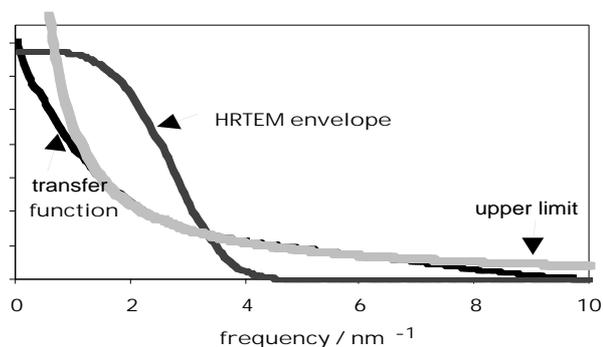


Fig. 4. The incoherent transfer function compared with that for HRTEM at a defocus spread of 30 nm.