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FFT MULTISLICE APPROACH FOR STEM IMAGE SIMULATION

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A new practical scheme for a STEM image simulation based on the FFT multislice algorithm has been developed[1]. This is applicable to simulate a high-angle annular dark-field (HAADF) STEM technique, which gives an image resolving atomic columns. Here, a HAADF intensity due to thermal diffuse scattering (TDS) is calculated from the absorptive potential corresponding to high-angle TDS and the wave function equivalent to the propagating probe within the sample. Although our scheme uses the same basic formula as used by Pennycook and Jesson[2] for a Bloch wave approach, a coherent bright-field intensity and a coherent HAADF intensity are also obtained straightforwardly.

The HAADF image contrast has been calculated for GaAs [011] to demonstrate its applicability. A matrix of 512x512 is used to sample a super cell made from 12x8 unit cells of GaAs [011], which extends over 4.80 by 4.51 nm. The sampling interval in real space then corresponds to about 0.01 nm, and the Fourier space extends up to almost 50 nm^{-1} with a sampling interval of about 0.2 nm^{-1}. A scanning scheme will be selected from an area, line and point modes and a scanning interval can be arbitrarily specified. A computation time on a personal computer is about 1 min for each scanning point calculated for 50 slices. In the case of GaAs then the area scan with a scanning interval of about 0.01 nm takes about 11 hours, which scans 21x29 points within an asymmetric area of the image symmetry *cm*. The HAADF images simulated for a 200kV microscope with Cs = 0.5 mm do not change so much their appearances up to 20-nm thickness except an overall growth of the signal strength as well as the background. However, the contrast of GaAs is not simply proportional to Z^2 as expected from Rutherford scattering at high-angle, and the As/Ga contrast ratio depends on the specimen thickness as shown in Fig. 1. This suggests that the generation of the HAADF signal is appreciably affected by the coherent dynamical scattering. Fig.1 also shows that the contrast depends on thermal displacement factors. Thus, the quantitative analysis requires a knowledge of the thermal displacement factors.

Next, we investigate an expected high-resolution STEM image that will be obtained by using a microscope equipped with a spherical aberration corrector. We assume here a hypothetical Cs-corrected 200 kV microscope with C_5 = 100 mm. Since the distance between the gallium and arsenic column in the dumbbell is 0.141 nm in [011] orientation, gallium and arsenic columns therefore will be easily resolved under the Cs-corrected conditions. The HAADF and the bright-field images simulated for GaAs [011] are reproduced in Fig.2. The appearances of HAADF images as well as the bright-field images do not change so much up to 20-nm thickness shown here.

The developed procedure will have a definitive advantage over the Bloch wave approach for simulating the HAADF images of a defect and interface or amorphous materials, and also the HAADF image obtained by using a Cs-corrected microscope. This is because the former requires a huge super cell, while the latter needs a large objective aperture including a large number of incident beam directions.

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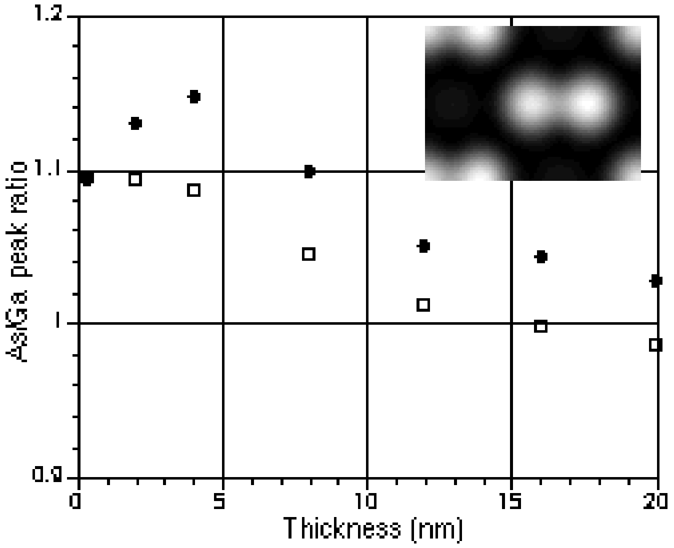

Figure 1 Contrast ratio of As/Ga as a function of specimen thickness. The HAADF images are calculated for two sets of the displacement parameters. Squares and dots show the contrast ratios obtained for the theoretical estimates (0.637 and 0.685 Å^2 for Ga and As) and the measured displacement values (0.687 and 0.568 Å^2 for Ga and As), respectively[3].

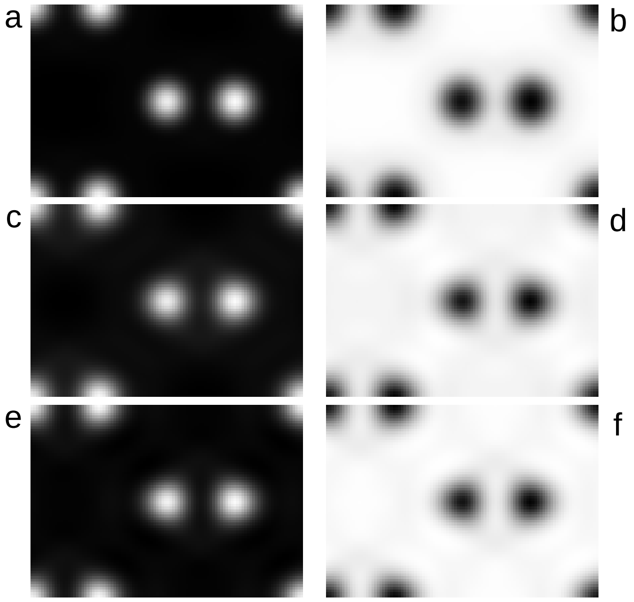

Figure 2 HAADF and bright-field images simulated for GaAs [011] under the Cs-corrected conditions. An objective aperture is set to 28.0 mrad. An annular dark-field detector extends between 56 and100 mrad, and the bright-field detector subtends to 28.0 mrad. The specimen thicknesses for (a, b), (c, d) and (e, f) correspond to 4.0, 12.0 and 20.0 nm, respectively.

References

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