Extraction of Quantitative Information from Non-optimum-focus Aberration-corrected HRTEM Images by Image Processing

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Aberration-corrected HRTEM images are expected to be taken under the optimum defocus (Δf_{opt}) condition to correctly reflect the crystal projected structure. However, the corrected state is intrinsically unstable, particularly when acquiring images at a resolution near the microscope information limit [1]. Moreover, the real defocus values are uncertain at the regions of interest away from the specimen edge, where the minimal contrast criterion for Gaussian focus can be applied. These factors can cause the image focus to deviate several nanometers from Δf_{opt}. This deviation can have a significant impact on quantitative analysis of HRTEM images, because of image distortions caused by modulation of the contrast transfer function (CTF). For these non-optimum focus images, image processing methods, such as exit-wave reconstruction [2] and image deconvolution [3], can be used to eliminate image distortion and restore the corresponding structure images.

Figure 1 shows the zincblende structure of $3C$-SiC and its [110] projection. The closely-spaced pairs of atomic columns of C and Si (called "dumbbells") with the separation distance of 1.09 Å are shown in Fig. 1(b). The multislice method was used to calculate series of non-optimum-focus aberration-corrected images for SiC [110] with varied Si or C atomic occupancies and slice thickness of 0.154 nm. The imaging parameters used for calculation were accelerating voltage U = 300 keV, instrumental information limit δ = 0.8 Å, specimen thickness t = 1.1 nm with positive C_S (C_S = 10 μm and Δf = −8 nm) and negative C_S (C_S = −10 μm and Δf = 3 nm) conditions, respectively. Figure 2(a) shows the CTF curves for these two conditions comparing with the Δf_{opt} (ｍ5 nm) conditions. Figure 2(b) shows a schematic diagram of ten independent diffraction beams with spatial frequencies below 1.25 Å^{-1}. None of the diffracted beams fall at the zero crossovers of the phase CTF curves. After performing deconvolution processing, the structure images restored from the non-optimum-focus images [Figs. 3(a) and (b)] for SiC [110] with full atomic occupancy are shown in Figs. 3(c) and (d), respectively. All atomic columns appear black and the SiC dumbbells are clearly visible. The restored structure images for SiC [110] with varied atomic occupancies are shown in Figs. 4(a)–(d). The C or Si occupancy of the center dumbbells (indicated by the hollow arrows) is varied from zero (left image) to full occupancy (right image) in steps of 0.2, respectively. The image contrast profiles across the center dumbbell positions along the $[00\bar{1}]$ direction (indicated by the solid arrow) from 0.1 to full C (or Si) occupancy in steps of 0.1 are shown in Figs. 4(e)–(h), respectively. These show that the image contrast of C (or Si) atomic columns increases with the C (or Si) content. Thus, the image processing technique can be regarded as a useful supplementary tool for aberration-corrected microscopes to extract quantitative information on the atomic scale [4].

References:
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[3] F.H. Li, *Phys. Status Solidi A* 207 (2010) 2639.
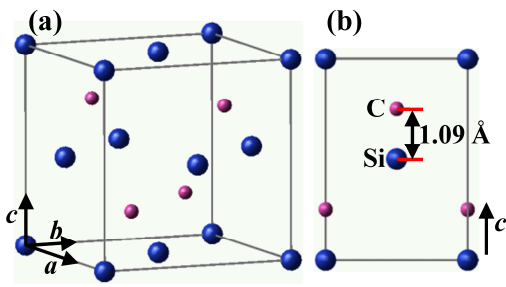[4] The work was supported by the State Scholarship Fund of China from China Scholarship Council.

Figure 1. Crystal structure of 3*C*-SiC in perspective view (a), and in projection along the [110] direction (b).
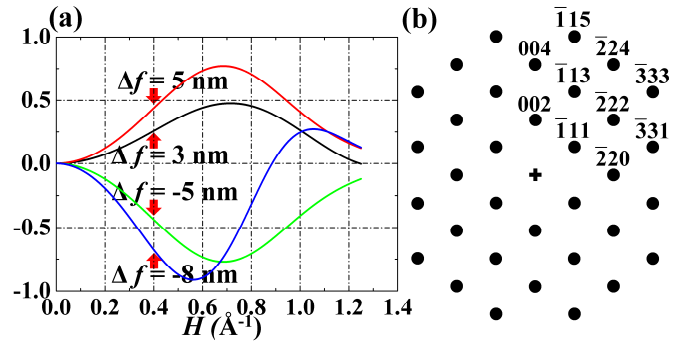

Figure 2. (a) CTF curves for C_S = 10 μm, Δf = −5, −8 nm and C_S = −10 μm, Δf = 3, 5 nm. (b) Schematic diagram of diffracted beams for 3*C*-SiC [110].

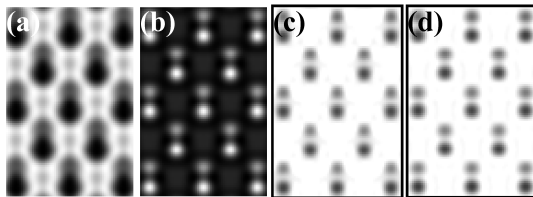**Figure 3.** Simulated non-optimum-focus images with t = 1.1 nm and (a) C_S = 10 μm, Δf = −8 nm, (b) C_S = −10 μm, Δf = 3 nm. (c) and (d) Restored structure images corresponding to (a) and (b), respectively.
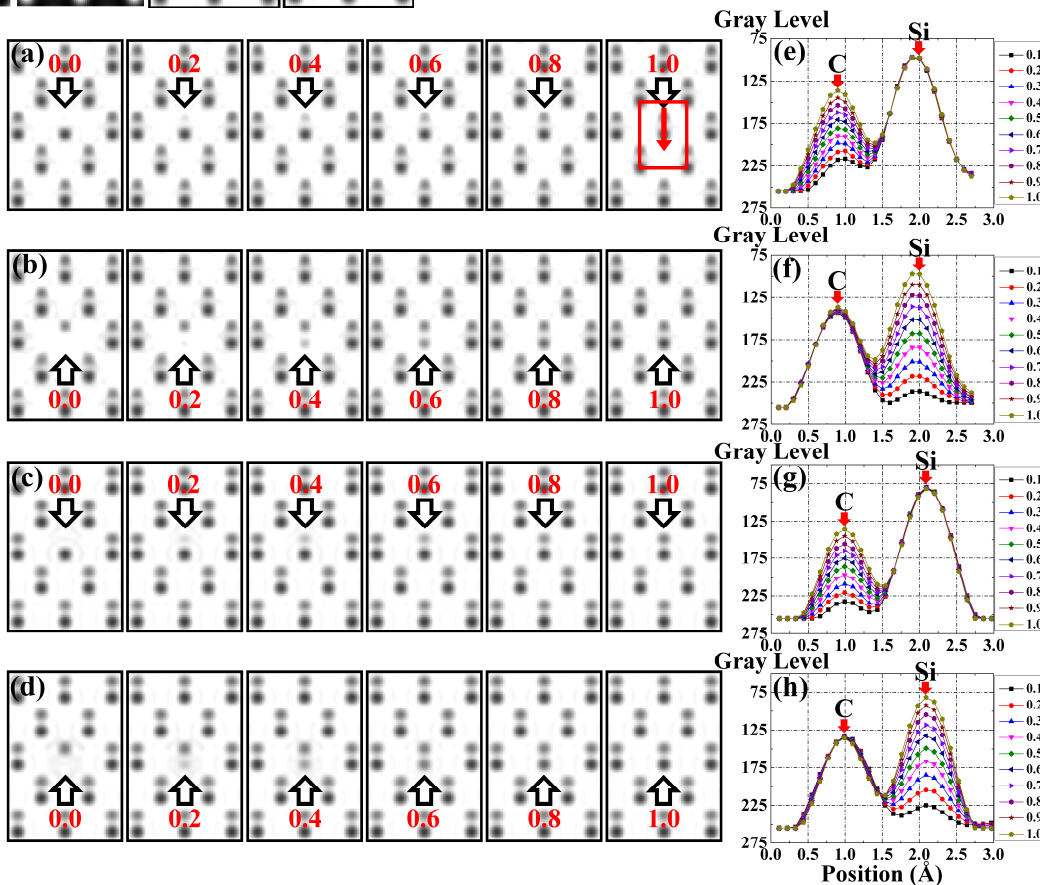

Figure 4. Restored structure images for SiC [110] with t = 1.1 nm, C_S = 10 μm, Δf = −8 nm [(a) and (b)] or C_S = −10 μm, Δf = 3 nm [(c) and (d)]. The C [(a) and (c)] or Si [(b) and (d)] occupancy of the center atomic column is varied from zero (left image) to full occupancy (right image) in steps of 0.2. (e)−(h) Image contrast profiles across the atomic columns along $[00\bar{1}]$ varying from 0.1 to full C or full Si occupancy in steps of 0.1, corresponding to (a)–(d), respectively.