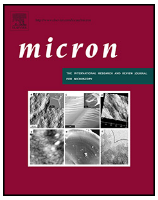
Micron 89 (2016) 77–86

Contents lists available at ScienceDirect

Micron

journal homepage: www.elsevier.com/locate/micron



Impact of dynamical scattering on quantitative contrast for aberration-corrected transmission electron microscope images

C. Wen[a,b,*], David J. Smith[b]

[a] *School of Science, Southwest University of Science and Technology, Mianyang 621010, China*
[b] *Department of Physics, Arizona State University, Tempe, AZ 85287, USA*

ARTICLE INFO

Article history:
Received 15 June 2016
Received in revised form 22 July 2016
Accepted 23 July 2016
Available online 25 July 2016

PACS:
68.37.Og
61.05.J–
81.70.Jb
42.30.Va

Keywords:
Aberration-corrected transmission electron microscopy
Dynamical scattering
Image contrast
Atomic-column position
Atomic occupancy
3*C*-SiC

ABSTRACT

Aberration-corrected transmission electron microscope images taken under optimum-defocus conditions or processed offline can correctly reflect the projected crystal structure with atomic resolution. However, dynamical scattering, which will seriously influence image contrast, is still unavoidable. Here, the multislice image simulation approach was used to quantify the impact of dynamical scattering on the contrast of aberration-corrected images for a 3*C*-SiC specimen with changes in atomic occupancy and thickness. Optimum-defocus images with different spherical aberration (C_S) coefficients, and structure images restored by deconvolution processing, were studied. The results show that atomic-column positions and the atomic occupancy for SiC 'dumbbells' can be determined by analysis of image contrast profiles only below a certain thickness limit. This limit is larger for optimum-defocus and restored structure images with negative C_S coefficient than those with positive C_S coefficient. The image contrast of C (or Si) atomic columns with specific atomic occupancy changes differently with increasing crystal thickness. Furthermore, contrast peaks for C atomic columns overlapping with neighboring peaks of Si atomic columns with varied Si atomic occupancy, which is enhanced with increasing crystal thickness, can be neglected in restored structure images, but the effect is substantial in optimum-defocus images.

1. Introduction

Transmission electron microscopes are powerful tools to study both qualitative and quantitative materials characteristics. The former provides determination of crystal structure, while the latter allows measurement of nanoscale (or smaller) materials parameters, such as atomic displacements, elemental distributions, and local component concentration. The early stages of quantitative high-resolution transmission electron microscopy (HRTEM) study were affected not only by insufficient microscope resolution, but also by imaging distortions due to dynamical scattering and modulation by the contrast transfer function (CTF). These effects seriously impact the extraction of quantitative information at the atomic scale (Kret et al., 2001).

Aberration-corrected transmission electron microscopes (Haider et al., 1998a,b; Smith, 2008) can enable quantitative HRTEM at the atomic scale. Compared to high-resolution scanning transmission electron microscopy, HRTEM allows much shorter image acquisition times and higher signal-to-noise ratio. The former reduces the effects of external disturbances at the time of recording images, and helps to avoid the impact of image drift. The latter enhances the ability to see weak, but often significant, changes of image contrast, such as in defective specimen regions (Tang and Freitag, 2004). Moreover, the negative spherical aberration imaging (NCSI) technique (Jia et al., 2010), which can result in even stronger image contrast for light elements, has been used frequently in quantitative HRTEM.

Although aberration-corrected HRTEM images taken under optimum-defocus (Δf_{opt}) conditions or after image processing (Kirkland and Meyer, 2004; Li, 2010) can eliminate image distortions caused by CTF modulation, dynamical scattering is still unavoidable. For quantitative HRTEM, analysis of the image contrast is critical because it can be used to determine atomic-column positions (corresponding to positions of contrast peaks), elemental distributions, and local component concentrations (the contrast is sensitive to atomic number and the number of atoms in an atomic column). It is known that the image contrast changes differently

---

[*] Corresponding author at: School of Science, Southwest University of Science and Technology, Mianyang 621010, China.
E-mail address: wencai@swust.edu.cn (C. Wen).

http://dx.doi.org/10.1016/j.micron.2016.07.008
0968-4328/

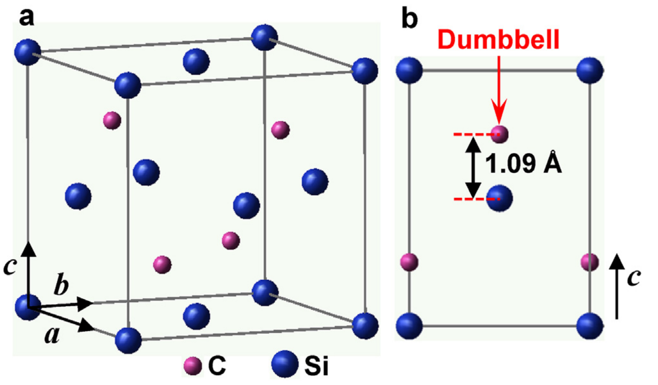


Fig. 1. 3*C*-SiC Crystal structure in perspective view (a), and in projection along the [110] direction (b).

with specimen thickness (t) for differently weighted (atomic number) atoms because of dynamical scattering (Tang et al., 1986; Tang et al., 2007; Wen et al., 2009, 2010, 2015; Cui et al., 2013). Unfortunately, this characteristic can only be used for distinguishing atomic species. Thus, the impact of dynamical scattering on quantitative interpretation of aberration-corrected images is still often unclear. Here, to research this problem, the multislice image simulation approach (Cowley and Moodie, 1957) has been used for a specimen of 3*C*-SiC. Changes in atomic occupancy and specimen thickness were studied for optimum-defocus images with positive and negative C_S coefficient, and structure images restored by processing images recorded at non-optimum defocus.

2. Material and methods

2.1. Crystal structure of 3C-SiC

3*C*-SiC has the zincblende structure, a common crystal structure in compound semiconductors, with a lattice parameter of 4.36 Å. Fig. 1a shows the 3*C*-SiC crystal structure in perspective view, and Fig. 1b shows a projection along the [110] direction. The closely-spaced pairs of C and Si atomic columns with the separation distance of 1.09 Å in projection are shown in Fig. 1b. Such atomic-column pairs are commonly called “dumbbells” in HRTEM. The reasons for selecting 3*C*-SiC to study are that many crystal structures can be resolved at atomic scale with image resolution of 1 Å, and image characteristics for light elements, such as carbon, are important in quantitative HRTEM.

2.2. HRTEM image simulation procedures

All HRTEM images were calculated using the multislice image simulation approach with the electron beam parallel to the [110] zone axis and a slice thickness of 1.54 Å (half of unit cell length along [110]). The atomic occupancies of Si ($O_{\rm Si}$) and C ($O_{\rm C}$) were varied from 0.1 to full occupancy in steps of 0.1. Imaging parameters were assigned by referring to the most common aberration-corrected electron microscopes with accelerating voltage (U) of 300 kV, defocus spread due to chromatic aberration (D) of 2.1 nm, and instrumental information limit of 0.08 nm. To provide minimum contrast delocalization and maximum phase contrast simultaneously, the $\Delta f_{\rm opt}$ can be set as $\mp\left(16/9\right)\left(\lambda g_{\max}^2\right)^{-1}$ with $C_S = \pm\left(64/27\right)\left(\lambda^3 g_{\max}^4\right)^{-1}$ (where underfocus and overfocus values correspond to positive and negative C_S coefficients, respectively), where λ is the electron wavelength, and $g_{\max}$ is the spatial frequency of instrumental information limit (Lentzen et al., 2002; Jia et al., 2004). Thus, optimum-defocus images were simulated with $\Delta f_{\rm opt} = \mp 5$ nm and $C_S = \pm 10$ µm in this work.

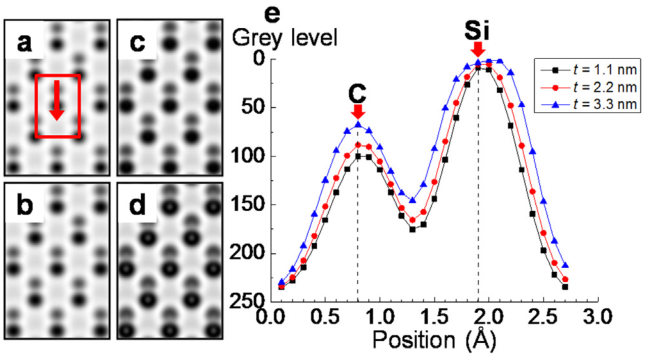


Fig. 2. Simulated optimum-defocus images for SiC [110] with C_S = +10 µm, Δf = −5 nm, and t of (a) 1.1 nm, (b) 2.2 nm, (c) 3.3 nm, and (d) 4.4 nm, (e) contrast profiles for the center SiC dumbbells in (a)–(c). The rectangle frame and line arrow in (a) mark a unit cell, and the position and [00$\bar{1}$] direction for image contrast measurement, respectively. Vertical dotted lines mark peak positions of C and Si atomic columns.

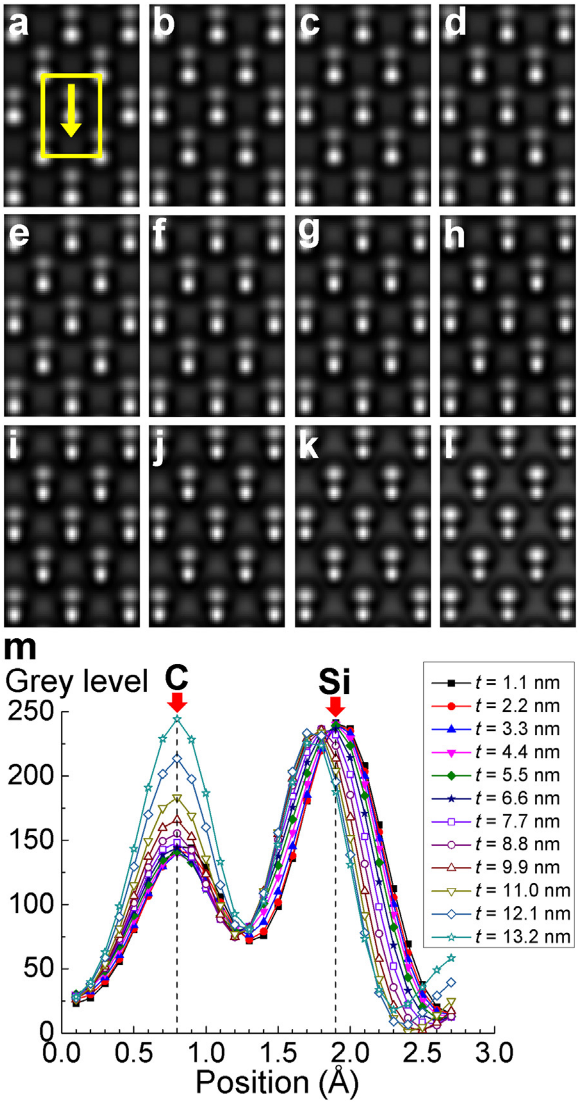


Fig. 3. Simulated optimum-defocus images for SiC [110] with C_S = −10 µm, Δf = +5 nm, and t increasing from (a) 1.1 nm to (l) 13.2 nm in steps of 1.1 nm, (m) contrast profiles for the center SiC dumbbells in (a)–(l). The rectangle frame and line arrow in (a) mark a unit cell, and the position and [00$\bar{1}$] direction for image contrast measurement, respectively. Vertical dotted lines mark peak positions of C and Si atomic columns.