Monte Carlo Study of the Influence of Electron Beam Focusing to SEM Image Sharpness Measurement*

Z. Ruan and P. Zhang
Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, University of Science and Technology of China, 96 Jinzhai Road, Hefei, Anhui 230026, P.R. China

S. F. Mao
School of Nuclear Science and Technology, University of Science and Technology of China, 96 Jinzhai Road, Hefei, Anhui 230026, P.R. China

H. M. Li
Supercomputing Center, University of Science and Technology of China, Hefei, Anhui 230026, P.R. China

Z. J. Ding†
Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, University of Science and Technology of China, 96 Jinzhai Road, Hefei, Anhui 230026, P.R. China.

(Received 9 January 2014; Accepted 20 March 2014; Published 31 May 2014)

The influence of electron beam focusing to SEM image sharpness has been studied by a Monte Carlo simulation method and an electron probe focusing model. The Monte Carlo simulation of the SEM image is based on a well-developed physical model of electron-solid interaction, which employs Mott’s cross section and a dielectric functional approach for electron elastic and inelastic scattering, respectively. A series of simulated SEM images for a practical sample, gold particles on a carbon substrate, are generated for different electron beam focusing conditions. For sharpness measurement three methods recommended by ISO/TS 245697 are used. The variation of image sharpness with the electron beam focusing condition is studied in detail.

[DOI: 10.1380/ejssnt.2014.247]

Keywords: Scanning electron microscope; Electron beam focusing; Monte Carlo; Image sharpness

I. INTRODUCTION

Sharpness is a key parameter for qualifying the performance of a scanning electron microscope (SEM). Many efforts have been put on the study of sharpness measurement methods. Some earlier work have initially defined the sharpness criterion and clearly demonstrated that image sharpness could be measured repeatedly [1–5]. For the purpose of measuring SEM sharpness in an objective and automatic way, several numerical methods have been proposed, e.g. Fourier transform (FT) method [6], autocorrelation function (ACF) method [7], derivative (DR) method [8, 9] and contrast-to-gradient (CG) method [10, 11]. At present these methods are considered useful for SEM image sharpness measurement; among them FT, DR and CG methods are recommended by ISO/TS 245697 [12], in which the sharpness of an SEM image is defined as “the minimum distance between two neighboring particles that can just be resolved”. Simulated SEM images generated by Monte Carlo method, with fully known parameters, have been demonstrated to be used for the sharpness measurement programs testing [13].

Generally, SEM image sharpness is limited by the fact that signal electrons collected for an individual pixel in SEM image are actually generated in a spread area instead of an ideal point. This actual spot diameter is initially affected by the electron source, aberrations and the amount of demagnification provided by the lenses. In a simplified electron beam focusing modeling, the spread is dominated by imperfect focusing of the final lens and a finite volume for beam-sample interaction [14]. A Gaussian probe shape is usually assumed to represent the primary electron beam profile [15]. However, the real beam shape at different landing positions of the beam on a sample structure could be quite different. The simulation results of Zhang et al. [16] have shown that the electron beam profile is deviated from the Gaussian probe shape because of the surface topography.

Cizmar et al.’s work [15] has provided repeatable computed SEM images with priori determined parameters by a rapid artificial image modeling using a series of equations and adjustable parameters. However, as the simple artificial image modeling has not taken account of the physical process of electron-solid interaction, the artificial image is independent of sample property and electron beam condition. Further work is therefore still needed based on our full understanding about beam-sample interaction. Monte Carlo simulation is a powerful tool for study of electron-solid interaction and secondary electron generation [17–19], while modeling of sample topography can be naturally included [20, 21]. By introducing finite element triangle mesh modeling [22, 23], Monte Carlo simulation has been improved to accommodate samples in arbitrary topography. This technique enables us to perform
image simulation for more realistic samples, e.g. irregular shaped gold particles on carbon substrate. It should be noted that, instrumental conditions are time dependent so that the repeatability of a real SEM is limited [13]. Instead of carrying out practical experiments, the repeatability can be guaranteed in an artificial computer experiment performed with a Monte Carlo simulation.

In this paper, we construct a more realistic modeling of SEM imaging by including further electron beam focusing, a dominate factor for the image sharpness. Monte Carlo simulation of beam-sample interaction for realistic sample topography and electron beam focusing has been performed to generate systematically a series of SEM images. The simulated images are then numerically evaluated by the three sharpness measurement, i.e. FT, CG and DR methods, specified by ISO/TS 245697 [12]. The influence of electron beam focusing to SEM Image sharpness measurement is studied.

II. ELECTRON BEAM FOCUSING MODELING

The landing spot size of an electron beam strongly depends on the focusing position, aperture angle and specimen structure [24]. Our model of the electron beam focusing is displayed in Fig. 1, in which \( \alpha \) represents the aperture angle and \( d_f \) describes the electron beam focusing distance measured from the substrate surface (\( d_f > 0 \) denotes the under-focus and \( d_f < 0 \) the over-focus). Focusing point is broadened into a disk with a diameter \( d_p \), which specifies the electron beam size due to the aberration of the objective lens. This modeling has been used to study the influence of electron beam focusing to SEM linewidth measurement [16] and is considered to be an effective method for simulation of beam focusing effect in SEM. In this work, we fixed the \( d_p \) value as 2.0 nm, according to the usual electron beam size in SEM operation. The aperture angle \( \alpha \) and the focusing distance \( d_f \) were set as two adjustable parameters for electron beam focusing condition. The ranges of the parameters were set according to the practical experimental requirements.

III. MONTE CARLO MODELING OF SEM IMAGING

A. Physical Model

For the complex scattering and transport processes of electrons in a solid sample, Monte Carlo method has been proven to be a powerful tool in the study of electron-solid interaction. In previous works we have studied secondary electron yield, energy spectra and SEM imaging [17–19]. By a Monte Carlo simulation, electron-solid interaction process is described by a series of discrete elastic and inelastic scattering events. Here we shall only briefly describe the elements of physical modeling, i.e. electron elastic scattering, electron inelastic scattering and cascade secondary electron generation.

Mott’s cross section [25] is used to describe electron elastic scattering. The relativistic representation of the differential elastic scattering cross section is given by

\[
\frac{d^2\sigma_e}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2,
\]

where \( |f(\theta)| \) and \( |g(\theta)| \) are scattering amplitudes:

\[
f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} \left\{ (l+1) \left( e^{i\delta_l^+} - 1 \right) + l \left( e^{i\delta_l^-} - 1 \right) \right\} \times P_l(\cos \theta),
\]

\[
g(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} \left\{ e^{-i\delta_l^+} + e^{i\delta_l^-} \right\} P_l^1(\cos \theta),
\]

\( \hbar k \) is the electron momentum, \( P_l(\cos \theta) \) and \( P_l^1(\cos \theta) \) are the Legendre and the first order associated Legendre functions, and \( \delta_l^+ \) and \( \delta_l^- \) are spin-up and spin-down phase shifts of the \( l \)-th partial wave, respectively.

In a dielectric function theory the differential cross section for electron inelastic scattering is given by:

\[
\frac{d^2\lambda_n^{-1}}{d\omega dq} = \frac{\hbar}{\pi a_0 E} \text{Im} \left\{ \frac{1}{\varepsilon(q, \omega)} \right\} \frac{1}{q},
\]

where \( a_0 \) is the Bohr radius and \( \hbar \) is Planck constant, \( h \omega \) and \( h q \) are respectively energy loss and momentum transfer. \( E \) is the kinetic energy of a moving electron. \( \text{Im}\{1/\varepsilon(q, \omega)\} \) and \( \varepsilon(q, \omega) \) are respectively the energy loss function and dielectric function of a solid. For calculating energy loss function, Penn has proposed an extrapolation scheme [26]:

\[
\text{Im} \left\{ \frac{1}{\varepsilon(q, \omega)} \right\} = \int_0^\infty d\omega_p g(\omega_p) \text{Im} \left\{ \frac{1}{\varepsilon_L(q, \omega; \omega_p)} \right\},
\]

where the expansion coefficient \( g(\omega) \) can be deduced from optical energy loss function.

In the inelastic scattering event, energy loss is transferred from the moving electron to a solid; thus, cascade secondary electrons would be generated in the successive inelastic scattering events for the generated electrons. The process of cascade secondary electron production has also been included in our Monte Carlo simulation.
B. Sample Topography

In Monte Carlo simulation of a realistic beam-sample interaction process, it is crucial to have a robust modeling of arbitrary sample topography. Because it is generally hard to have an analytical representation of a real sample surface, a finite element mesh modeling [27] can be employed, with which an arbitrary sample surface can be approximated by many small triangle planes. A detailed description of this finite element mesh modeling together with space subdivision and linear space generation method for accelerating simulation has been described elsewhere [22, 23].

IV. SEM IMAGE SHARPNESS MEASUREMENT METHODS

Three methods recommended by ISO/TS 245697:2011 [12], i.e. FT method, CG method and DR method, were used to evaluate the sharpness of SEM images. The general idea behind these methods is to find an optimal convoluted image which almost agrees with the original SEM image; the convoluted image is obtained by a convolution of a 2D Gaussian profile with the binary segmentation of the SEM image.

The FT method compares the Fourier transformed 2D intensity profiles of an SEM image with those of the convoluted images with different sharpness factors. The CG method considers weighted harmonic mean gradients of the 2D brightness distribution map of an SEM image and the image sharpness is inversely proportional to the weighted harmonic mean of the gradients. The DR method is achieved by fitting error function profiles to gradient directional-edge profiles of particles in an SEM image and the image sharpness is derived from the average of the edge sharpness of all the edge slopes.

Considering possible different response behavior of the sharpness measured by the three methods to various experimental parameters, we have proposed to use a mean, simple average $\bar{S}$ or weighted average $\langle S \rangle$ as defined below, of three sharpness values as a candidate for an appropriate measure of SEM image sharpness [28],

$$ S = (S_{FT} + S_{CG} + S_{DR})/3 $$

$$ \langle S \rangle = \frac{1}{2} S_{FT} + \frac{1}{4} S_{CG} + \frac{1}{4} S_{DR}. $$

V. RESULTS

Gold particles on a carbon substrate sample is usually used for obtaining a SEM image of good contrast for sharpness measurement [1]. To study the beam-sample interaction in a realistic sample, Zhang et al. have constructed a gold-on-carbon sample topography by finite element mesh modeling according to a realistic SEM image [23]. This sample topography is used in the present work and the electron beam focusing model is taken into account to calculate SE images under different focusing cases. Simulations are performed for 1 keV primary beam at normal incidence. Simulated SEM images are of 256×256 pixels. All secondary electrons emitted from sample surface with energies lower than 50 eV are collected as secondary electron signal.

A series of Monte Carlo simulated SEM image under different focus conditions described by two parameters, focusing position $d_f$ and aperture angle $\alpha$, are obtained. Displayed in Fig. 2 are simulated SEM images at various focusing positions. The results indicate that when

FIG. 2: Monte Carlo simulated SEM images at various focusing positions, $d_f$: (a) 20 nm; (b) $-20$ nm; (c) 100 nm; (d) $-100$ nm. The aperture angle $\alpha$ is 42.5 mrad.

FIG. 3: Monte Carlo simulated SEM images for various aperture angles, $\alpha$: (a) 17 mrad; (b) 34 mrad; (c) 51 mrad; (d) 68 mrad. The focusing position $d_f$ is 0.0 nm.
the aperture angle remains the same, the image quality becomes worse with increasing the absolute defocusing distance measured from the substrate surface. And the under-focus ($d_f > 0$) and over-focus ($d_f < 0$) case affect the SEM image at almost the same level. Setting the focusing position $d_f$ as 0.0 nm, Fig. 3 shows simulated SEM images for various aperture angles. The edge effect of the gold particles is more visible in an image for smaller aperture angle, but it is obviously that the image quality changes little when the focusing position stays the same while the aperture angle increases.

Then the three sharpness measurement methods were used to calculate the sharpness values of the simulated SEM images described above. A mean, simple average $\bar{S}$ or weighted average $\langle S \rangle$ defined in Eq. (5) are obtained considering the different sharpness values measured by three methods. Figure 4 displays the sharpness value variation with focusing position, when the aperture angle is fixed at 42.5 mrad. And when the focusing position is set as 0.0 nm, the image sharpness is calculated for different aperture angles, as shown in Fig. 5. It is clearly that, the aperture angle hardly affects the image sharpness. But with the increasing of the absolute defocusing distance measured from the substrate surface, the image sharpness value measured by all the three methods gradually increases, indicating that the image quality gets worse. This result is consistent with the previous qualitative analysis of the simulated images.

VI. CONCLUSIONS

In conclusion, we have improved our Monte Carlo modeling for SEM image to include beam focusing condition. Considering that the real beam shape at different landing positions of the beam on a sample structure could be quite different, the traditional treatment of convolving an image under a zero diameter electron beam with a Gaussian probe shape is too rough. A more realistic electron beam focusing modeling has been introduced to our Monte Carlo modeling. The present simulation can be used to generate a series of SEM images for different instrumental parameters, representing more realistic beam and sample conditions. We have used the simulated images to evaluate different sharpness measurement methods including the recommended methods by ISO/TS 245697. The image sharpness measurement can quantitatively estimate the effect of electron beam focusing to the image quality in SEM.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (Nos. 11074232, 11274288 and 11204289), the National Basic Research Program of China (Nos. 2011CB932801 and 2012CB933702), Ministry of Education of China (No. 20123402110034), “111” project (No. B07033) and Chinese Academy of Sciences (No. XXH12503-02-02-07).

[1] M. T. Postek and A. E. Vladar, Scanning 20, 1 (1998).
[2] A. E. Vladar, M. T. Postek, and M. P. Davidson, Scanning 20, 24 (1998).
[3] N. F. Zhang, M. T. Postek, R. D. Larrabee, A. E. Vladar, W. J. Kerry, and S. N. Jones, Scanning 21, 246 (1999).
[4] N. F. Zhang, A. E. Vladar, M. T. Postek, and R. D. Larrabee, Metrologia 42, 351 (2005).
[5] N. F. Zhang, A. E. Vladar, M. T. Postek, and R. D. Larrabee, Proc. Section of Physical and Engineering Sciences of American Statistical Soc., 4730 (2003).
[6] D. C. Joy, J. Microsc. 208, 24 (2002).
[7] D. C. Joy, Y.-U. Ko, and J. J. Hwu, Proc. SPIE 3998, 108 (2000).
[8] J. Dijk, M. van Ginkel, R. van Asselt, L. van Vliet, and P.
Verbeek, in: Computer Analysis of Images and Patterns, Eds. N. Petkov and M. Westenberg (Springer, Berlin-Heidelberg, 2003), p. 149.

[9] B. Rieger and G. N. A. Veen, in EMC 2008 14th Electron Microscopy Congress, Vol. 1: Instrumentation and Methods, Eds. M. Luysberg, K. Tillmann, and T. Weirich (Springer, Berlin Heidelberg, 2008), p. 613.

[10] T. Ishitani and M. Sato, J. Elect. Microsc. 51, 369 (2002).
[11] T. Ishitani and M. Sato, J. Elect. Microsc. 56, 145 (2007).

ISO/TS 24597, “Microbeam analysis-Scanning electron microscopy-Methods of evaluating image sharpness”, 2011.

[12] M. T. Postek and A. E. Vladar, Scanning 33, 111 (2011).
[13] L. Reimer, Scanning Electron Microscopy: Physics of Image Formation and Microanalysis (Springer, Berlin-Heidelberg-New York, 1998).
[14] P. Cizmar, A. E. Vladar, B. Ming, and M. T. Postek, Scanning 30, 381 (2008).
[15] P. Zhang, S. F. Mao, Z. M. Zhang, and Z. J. Ding, Proc. SPIE 8729, 87290K (2013).
[16] Z. J. Ding and R. Shimizu, Scanning 18, 92 (1996).