Enhancement of spatial resolution in generating point spread functions by Monte Carlo simulation in electron-beam lithography

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The point spread function (PSF) plays an important role in electron beam lithography, e.g., for the estimation of the resist profile, proximity effect correction, etc. The conventional approach often derives PSFs directly from the Monte Carlo simulation, which might have a limitation in the spatial resolution under a certain size of memory available on a computer. A novel method is proposed to enhance the spatial resolution of PSFs generated from the Monte Carlo simulation without increasing the memory size or changing the simulation software. It exploits the fact that the PSF is radially symmetric and utilizes the concept of integrating the PSF. The integrated PSF is generated by the Monte Carlo simulation, and then the PSF is mathematically derived from its integration. Simulation results show that the proposed method has good potential for providing a practical way to enhance the spatial resolution of the PSF. © *2011 American Vacuum Society*.
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I. INTRODUCTION

In electron beam (e-beam) lithography, electron scattering is modeled by using a point spread function (PSF) that is radially symmetric and which shows how the electron energy is distributed throughout the resist when a single point is exposed. In general, PSFs are used to compute the exposure (energy deposited in the resist) distribution by convolution with a circuit pattern (dose distribution). Therefore, the quality of a PSF is crucial in applications such as proximity effect correction[1–5] and the estimation of remaining resist profiles.[6–9]

One of the widely used methods for generating PSFs in electron-beam lithography is to rely on the Monte Carlo simulation.[10–12] A substrate system including the resist layer is modeled as a three-dimensional (3D) array of (cubic) cells, and the random path of each electron is traced, with the electron energy being deposited in the cells along the path. The final contents of the cells are a 3D PSF sampled at the interval of the cell size. The spatial resolution, i.e., the size of a cell, depends on the size of the 3D array. A higher spatial resolution or a smaller cell requires a larger array. The maximum size of the array is determined by the size of the memory available on the computer being used. It is often the case that the desired resolution is not achievable due to the limited memory size, especially on a personal computer (PC).

In this study, a novel method for enhancing the spatial resolution of a PSF without increasing the size of the memory used or changing the simulation program has been developed based on the mathematical formulation. The idea of decreasing the dimensionality of the domain was exploited for a radially symmetric problem in signal processing.[13] In our proposed method, the main idea is to reduce one of the dimensions in the representation of the simulation space in order to increase the spatial resolution in the remaining dimension(s). The dimension is reduced by elongating the cell along the dimension, which is equivalent to integrating the 3D PSF along the dimension. Then, the PSF is derived mathematically from the integrated PSF obtained from the simulation. The increased resolution is maintained through the PSF derivation. The improvement of spatial resolution has been demonstrated through simulations using the software CASINO v2.42.[11]

The rest of the paper is organized as follows: The Monte Carlo simulation is briefly reviewed in Sec. II. The proposed method is described in detail in Sec. III. Simulation results are presented in Sec. IV and are followed by a summary in Sec. V.

II. MONTE CARLO SIMULATION

The Monte Carlo simulation is a widely used approach for deriving PSFs. It traces individual electrons, following paths that have been stochastically determined based on the phenomena and effects that have been theoretically modeled. The electron paths in a cross-section of the substrate system consisting of 300 nm PMMA on Si (with a beam energy of 10 keV), generated by the CASINO software, are shown in Fig. 1. The Monte Carlo simulation provides not only the electron paths, but also the energy distribution in the resist (and substrate), i.e., the PSF to be derived. The electron energies deposited in the cells are computed along each path. The energy distribution in the cross-section is shown in Fig. 2, where different grayscale levels denote different levels of the deposited energy. The accuracy of the PSFs generated by such a simulation depends on the theoretical model employed and the number of electrons traced. As long as the number of electrons is sufficiently large and all or most of the major phenomena and effects are modeled, the PSFs are considered to be accurate. Note that although the electron trajectories are illustrated in a cross-section in Fig. 1, the

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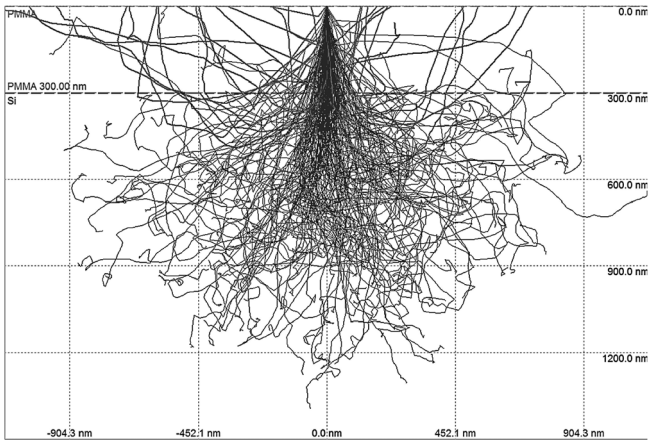

FIG. 1. Monte Carlo simulation of electron paths (cross-section).

actual simulation is carried out for a 3D space modeled by a 3D array.

III. PROPOSED METHOD

The key idea of the proposed method is to reduce the dimensionality in the representation of the simulation space and increase the spatial resolution in the remaining dimension(s). That is, the PSF is integrated along the dimension to be reduced (one of the x- and y-dimensions where the z-axis corresponds to the resist depth dimension) during the simulation. The PSF is derived from the integrated PSF mathematically, exploiting the fact that a PSF is radially symmetric. In this derivation, the increased spatial resolution is maintained.

A. Integration of PSF

Let $p[i][j][k]$ represent the 3D array or PSF where k corresponds to the resist (substrate) depth dimension as shown in Fig. 3(a). A 3D PSF may be considered as a stack of two-dimensional (2D) PSFs, where a 2D PSF is a layer of $p[i][j][k]$ with k fixed, to be denoted by $p_k[i][j]$ [see Fig. 3(c)]. In the proposed method, in order to increase the spatial resolution in the i dimension, the substrate system is modeled by a 2D array $P[i][k]$ obtained by elongating the cell (in $p[i][j][k]$) in the j dimension so that it is long enough to cover the electron scattering range, as shown in Fig. 3(b).

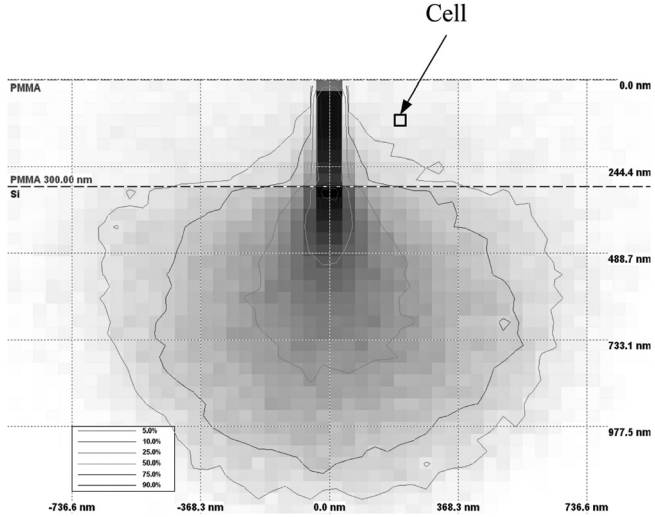

FIG. 2. Monte Carlo simulation of energy distribution (cross-section).

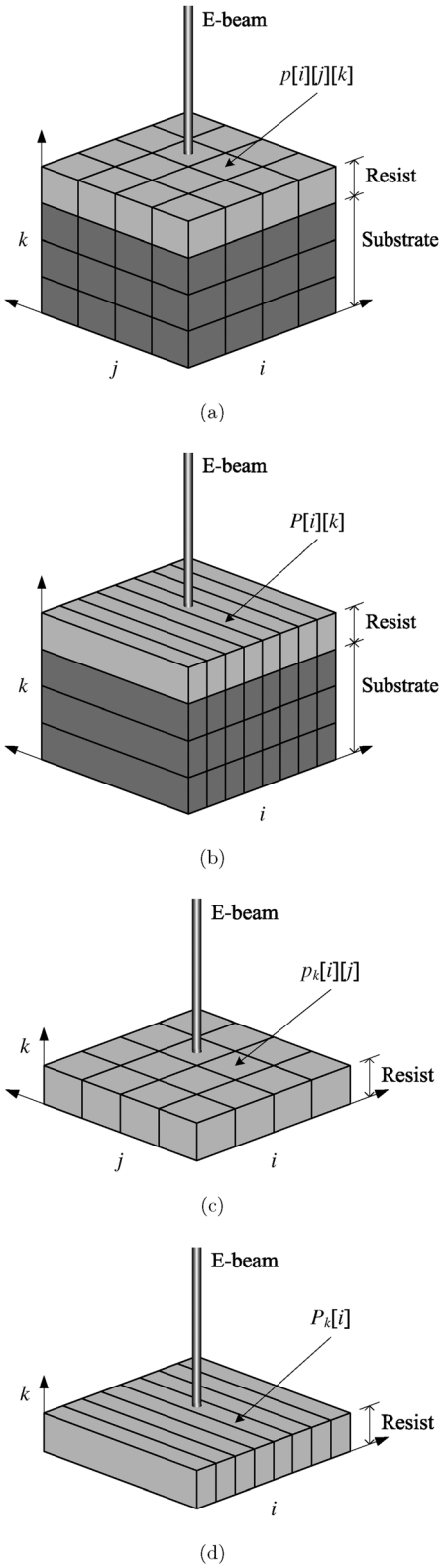

FIG. 3. Partitioning of simulation space: (a) 3D array of cubic cells $p[i][j][k]$, (b) 2D array of rectangular-pipe cells $P[i][k]$, (c) 2D array of cubic cells for a single layer $p_k[i][j]$, and (d) 1D array of rectangular-pipe cells for a single layer $P_k[i]$.

Then, $P[i][k]$ is the sum of exposures deposited in the cells corresponding to the set $\{p[i][j][k] \mid \text{all } j\}$, i.e.,

$$P[i][k] = \sum_j p[i][j][k]. \tag{1}$$

For a fixed k (e.g., a layer of resist), the same relationship can be established.

$$P_k[i] = \sum_j p_k[i][j], \tag{2}$$

where $P_k[i]$ is a 1D array representing the 2D simulation space as shown in Fig. 3(d). That is, $P[i][k]$ and $P_k[i]$ are the integrations of 3D and 2D PSFs along the j dimension, respectively. Note that more cells (equivalently smaller cells and therefore increased spatial resolution) can be allowed in the i dimension of $P[i][k]$ and $P_k[i]$, as the j dimension does not need to be represented. The relationship between $p_k[i][j]$ and $P_k[i]$ is illustrated in Fig. 4. A 3D PSF is a stack of 2D PSFs in which the layers of the 2D PSFs are independent of each other. Therefore, in the following sections, the proposed method is described for deriving a 2D PSF, $p_k[i][j]$, from its integration, $P_k[i]$.

B. Derivation of PSF from its integration

Because the 2D PSF can be considered radially symmetric in most cases (except when a stochastic model of PSF needs to be used), $p_k[i][j]$ may be replaced by a 1D array or PSF $p_k[l]$, where $p_k[i][j] = p_k[\sqrt{i^2 + j^2}]$. Then, $P_k[i]$ can be expressed, for each i, by a linear equation of the elements in the set $\{p_k[l] \mid l = 1,2,\cdots\}$, because in general $p_k[i][j]$ can be represented by a linear interpolation between two adjacent elements of $p_k[l]$ and $p_k[l+1]$. That is, a linear equation is formulated for each $P_k[i]$,

$$\begin{aligned} P_k[i] &= p_k[i] + 2 \cdot \sum_{s=1}^{\lfloor \sqrt{R^2 - i^2} \rfloor} p_k\left[\sqrt{i^2 + s^2}\right] \\ &= p_k[i] + 2 \cdot \sum_{s=1}^{\lfloor \sqrt{R^2 - i^2} \rfloor} ((\lfloor d \rfloor + 1 - d) \cdot p_k[\lfloor d \rfloor] \\ &\quad + (d - \lfloor d \rfloor) \cdot p_k[\lfloor d \rfloor + 1]), \end{aligned} \tag{3}$$

where $d = \sqrt{i^2 + s^2}$ and R corresponds to the electron scattering range.

The above summation to compute $P_k[i]$ can also be expressed in the form of matrix multiplication,

$$P_k = A \times p_k, \tag{4}$$

where P_k is the vector $(P_k[i] \mid i = 1,2,\cdots)$, p_k is the vector $(p_k[i] \mid i = 1,2,\cdots)$, and the element $A[i][l]$ of the matrix A quantifies how much $p_k[l]$ affects $P_k[i]$.

The element $A[i][l]$ can be derived by rearranging the terms in Eq. (3) as follows:

$$A[i][l] = \begin{cases} 0 & \text{for} \quad i > l \\ 1 + 2 \cdot \sum_{s=\lceil s_2 \rceil}^{\lfloor s_3 \rfloor} (\lfloor d \rfloor + 1 - d) + 2 \cdot \sum_{s=\lceil s_1 \rceil}^{\lfloor s_2 \rfloor} (d - \lfloor d \rfloor) & \text{for} \quad i = l \\ 2 \cdot \sum_{s=\lceil s_2 \rceil}^{\lfloor s_3 \rfloor} (\lfloor d \rfloor + 1 - d) + 2 \cdot \sum_{s=\lceil s_1 \rceil}^{\lfloor s_2 \rfloor} (d - \lfloor d \rfloor) & \text{for} \quad i < l \end{cases}, \tag{5}$$

where $s_1 = \sqrt{(l-1)^2 - i^2}$, $s_2 = \sqrt{l^2 - i^2}$, and $s_3 = \sqrt{(l+1)^2 - i^2}$.

As long as the sizes of the vectors p_k and P_k are the same, the square matrix A is invertible because A is an upper triangular matrix.

Then, the linear equations in Eq. (4) can be solved to derive the 1D PSF $p_k[l]$ from $P_k[i]$ by (refer to Fig. 5)

$$p_k = A^{-1} \times P_k. \tag{6}$$

Note that the spatial resolution of $p_k[l]$ is the same as that of $P_k[i]$.

Due to the fact that P_k is radially symmetric, A is an upper triangular matrix in which the size of each dimension is that of P_k. Therefore, the matrix inversion in Eq. (6) can be carried out via the Gaussian elimination algorithm. Furthermore, each row of A is loaded into memory individually for processing, starting from the last row, i.e., the ith row is loaded and $p_k[i]$ is solved (computed) before the $(i-1)$th row is loaded. In this way, the entire matrix A does not have to be loaded into memory. Thus, the size of the memory required for the inversion step is only that of P_k, which is no more than the size of the memory for the direct simulation.

The $P_k[i]$ generated by the Monte Carlo simulation tends to include oscillations, especially in the long-range part. The oscillations would be magnified through the process of solving the linear equations and would result in a noisy $p_k[l]$. Note that the matrix multiplication in Eq. (6) is equivalent to high-pass filtering. The proposed method employs a smoothing filter to remove those oscillations in $P_k[i]$; it is a moving average filter with which the window size is dependent on the location. The window size progressively increases blockwise as the distance from the origin increases. Also, depending on the PSF, it might be necessary to iterate this smoothing operation multiple times. For the results in this paper, the window size was 1 for the first 4 points, 5 for the

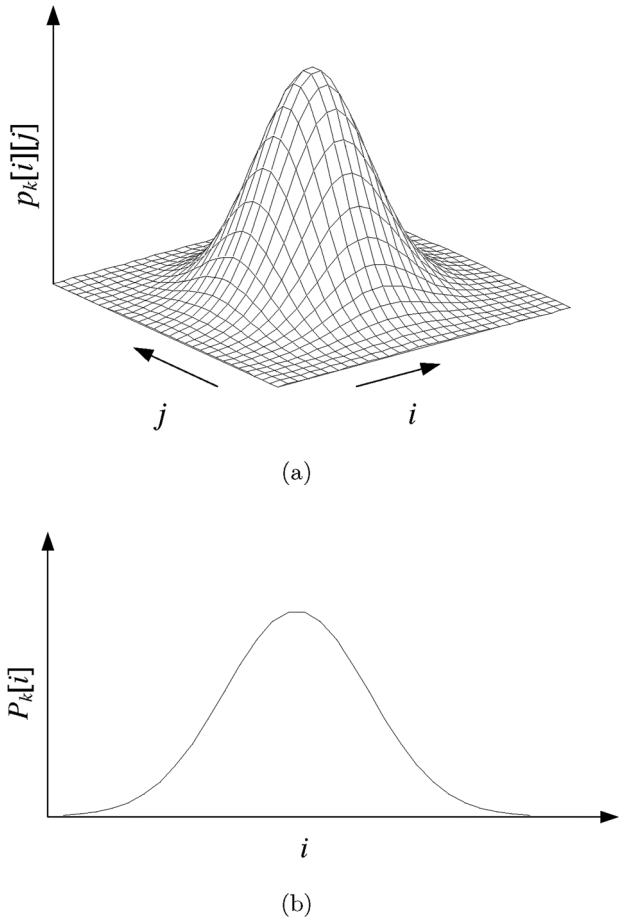

FIG. 4. Relationship between (a) $p_k[i][j]$ and (b) $P_k[i]$.

next 5 points, 10 for the next 40 points, and 50 for the rest, and the smoothing was iterated 10 times.

C. Procedures

The procedures followed in the proposed method are summarized below (also refer to the flow chart in Fig. 6).

Step 1: Represent the 2D simulation space (e.g., a resist layer) as a 1D array of long cells.

Step 2: Run the Monte Carlo simulation to obtain $P_k[i]$.

Step 3: Apply a smoothing filter to $P_k[i]$ to remove oscillations.

Step 4: Generate matrix A according to Eq. (5).

Step 5: Derive the PSF $p_k[l]$ from $P_k[i]$ by solving $A \times p_k = P_k$ through a Gaussian elimination algorithm.

IV. RESULTS AND DISCUSSION

A. Simulation results

The proposed method has been tested using the data generated from the Monte Carlo simulation by the CASINO software. The substrate systems employed in the simulation are composed of PMMA on Si with two different combinations of PMMA thickness and beam energy: 300 nm/50 KeV (referred to as substrate system I) and 500 nm/100 KeV (referred to as substrate system II). The beam diameter is 5

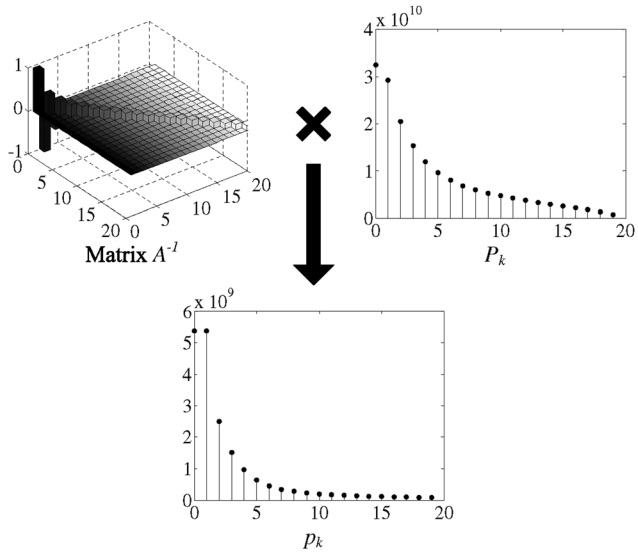

FIG. 5. $p_k[l]$ can be solved from $P_k[i]$ through matrix inversion and multiplication.

nm, and the number of electrons in the simulation is 1 000 000. The results are provided in Figs. 7–10. For substrate system I, the highest spatial resolution possible on a PC with 2 Gbytes is about 85 nm when the substrate system is modeled by a 3D array ($p[i][j][k]$, $400 \times 400 \times 400$). The accuracy of the proposed method has been examined for a spatial resolution of 85 nm by comparing the PSF [Fig. 7(b)] derived from $P_k[i]$ [Fig. 7(a)] via the proposed method to the PSF [Fig. 7(c)] directly generated from the CASINO software. A similar comparison is also made in Fig. 9 for substrate system II when the highest spatial resolution is about 287 nm under the same simulation specification. It is clear that the two PSFs match well [refer to Figs. 7(d) and 9(d)], indicating the high accuracy of the proposed method.

Modeling the substrate systems by a 2D array ($P[i][k]$, 8000×8000) improves the spatial resolution to about 4 nm for substrate system I and 14 nm for substrate system II, and the corresponding $P_k[i]$ are shown in Figs. 8(a) and 10(a), respectively. The PSFs with a spatial resolution of 4 nm for substrate system I and 14 nm for substrate system II, derived

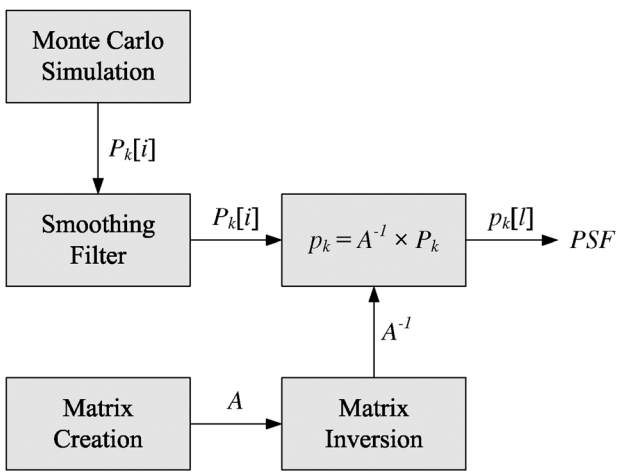

FIG. 6. Flow chart of the proposed method.

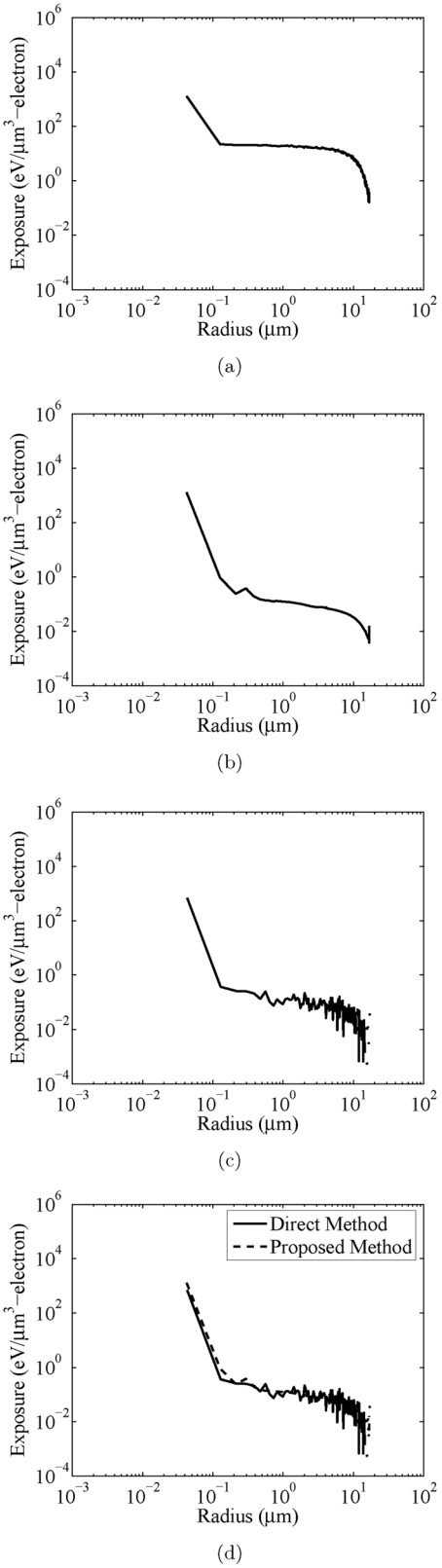

FIG. 7. Simulation results for 300 nm PMMA on Si with a beam energy of 50 KeV (spatial resolution ≈ 85 nm): (a) $P_k[i]$ generated by CASINO, (b) PSF ($p_k[l]$) derived from $P_k[i]$ via the proposed method, (c) PSF ($p_k[i][j]$) directly generated by CASINO, and (d) a comparison between the PSF derived via the proposed method and the PSF directly generated by CASINO.

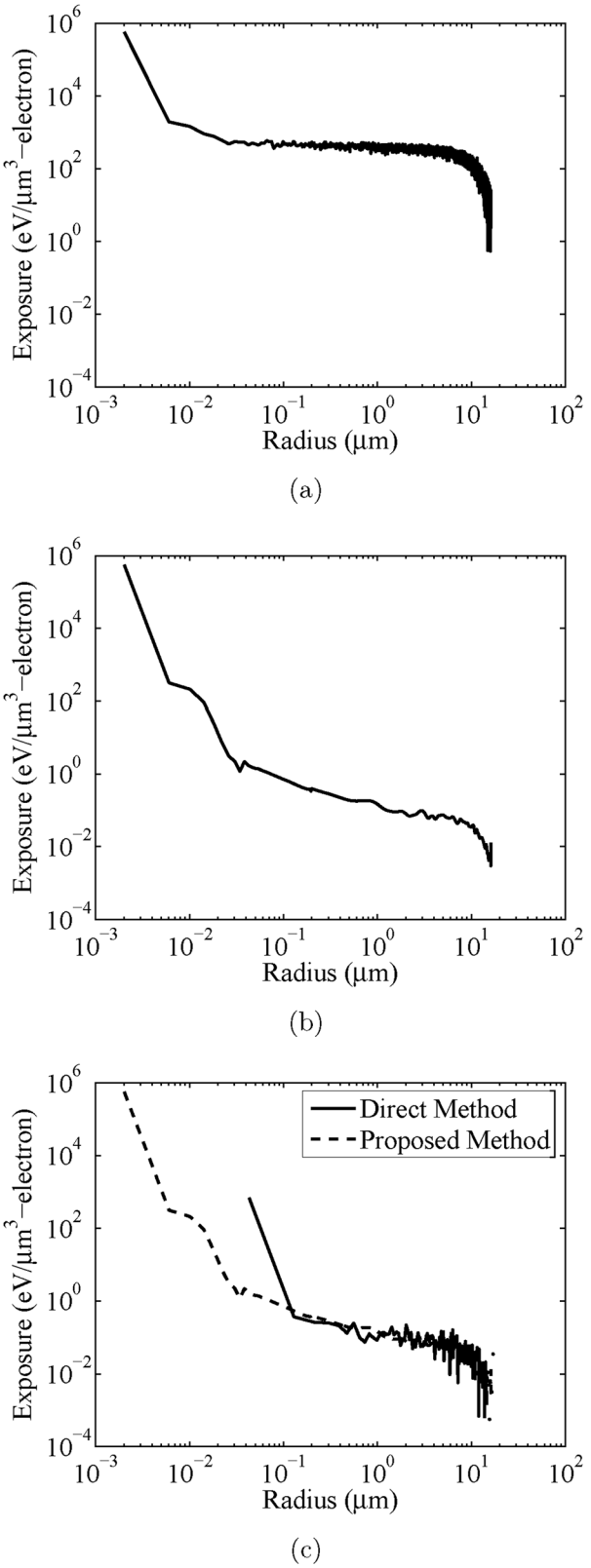

FIG. 8. Simulation results for 300 nm PMMA on Si with a beam energy of 50 KeV (spatial resolution ≈ 4 nm): (a) $P_k[i]$ generated by CASINO, (b) PSF ($p_k[l]$) derived from $P_k[i]$ via the proposed method, and (c) a comparison between the PSF derived via the proposed method and the PSF directly generated by CASINO.

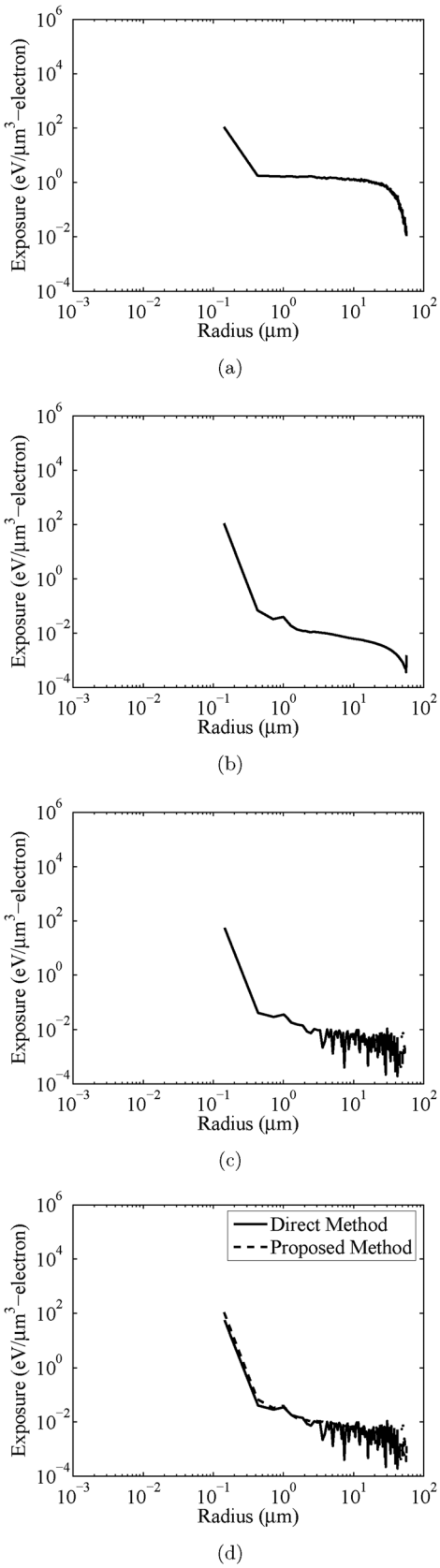

FIG. 9. Simulation results for 500 nm PMMA on Si with a beam energy of 100 KeV (spatial resolution ≈ 287 nm): (a) $P_k[i]$ generated by CASINO, (b) PSF ($p_k[l]$) derived from $P_k[i]$ via the proposed method, (c) PSF ($p_k[i][j]$) directly generated by CASINO, and (d) a comparison between the PSF derived via the proposed method and the PSF directly generated by CASINO.

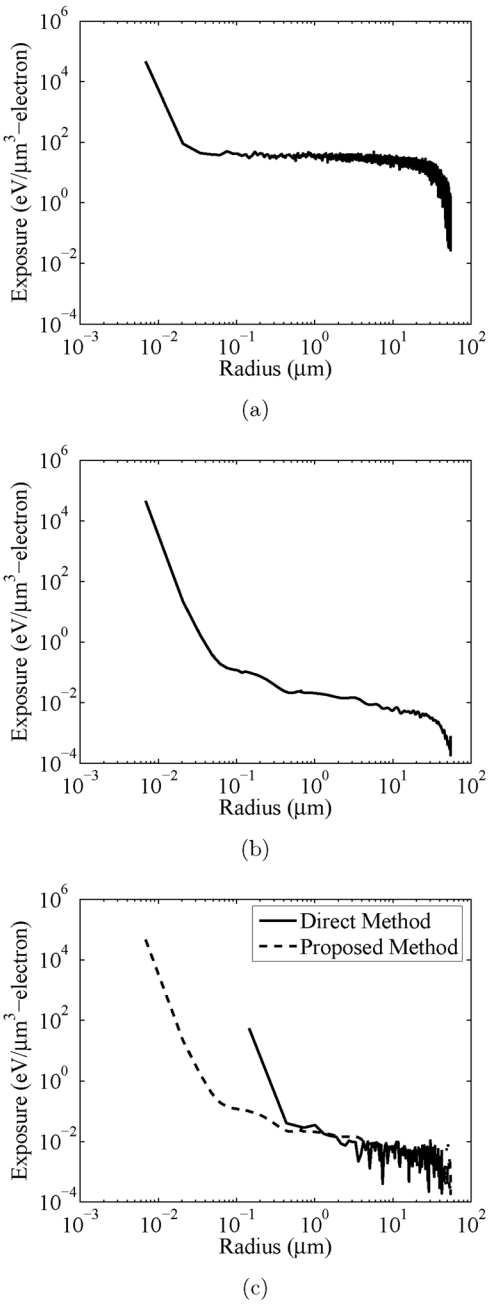

FIG. 10. Simulation results for 500 nm PMMA on Si with a beam energy of 100 KeV (spatial resolution ≈ 14 nm): (a) $P_k[i]$ generated by CASINO, (b) PSF ($p_k[l]$) derived from $P_k[i]$ via the proposed method, and (c) a comparison between the PSF derived via the proposed method and the PSF directly generated by CASINO.

via the proposed method, are provided in Figs. 8(b) and 10(b), respectively. From Figs. 8(c) and 10(c), it is seen that the high-resolution PSFs derived via the proposed method reveal more detail in the short range, i.e., the forward scattering part, where most of the deposited energy is concentrated. Note that on a PC with 2 Gbytes this high-resolution PSF cannot be generated directly from the Monte Carlo simulation using the 3D array $p[i][j][k]$.

The high-resolution PSFs shown in this paper are for the top 30% of resist, i.e., the energy deposited is integrated along the resist depth dimension over the top 2400

$(8000 \times 30\%)$ layers. Note that the thickness of one of the 8000 layers over the 300 nm thick PMMA is less than 0.04 nm $(=300\text{nm}/8000)$. Therefore, the signal-to-noise ratio in a layer is too low to derive a smooth (single-layer) PSF, unless the number of electrons is increased significantly or an excessive smoothing operation is employed in the derivation.

B. Memory reduction

The computation time added by the proposed method is very small compared to that of the Monte Carlo simulation. For the results reported in this paper, it is few minutes, whereas the simulation takes hours on a PC. Therefore, only the memory complexity is discussed below.

Suppose that $p[i][j][k]$ is of the size $n \times n \times n$ and $P[i][k]$ is of the size $N \times N$. If the size of the memory on a computer is M in terms of the number of cells, $n^3 = N^2 = M$. Then, $n = \sqrt[3]{M}$and $N = \sqrt[2]{M}$. The spatial resolution (defined as the size of a cell) achieved by the proposed method is proportional to $1/N = 1/\sqrt[2]{M}$, compared to $1/n = 1/\sqrt[3]{M}$ as obtained by the conventional method. That is, the spatial resolution is improved $\sqrt[6]{M}$ times by the proposed method, e.g., the resolution is 10 times higher when $M = 10^6$.

V. SUMMARY

A novel method for enhancing the spatial resolution of PSFs generated from Monte Carlo simulations is proposed in this paper. The proposed method reduces the dimensionality of the simulation space by equivalently integrating the PSF along a dimension in order to increase the resolution in the remaining dimension(s) during the simulation. The PSF is derived from the integrated PSF, with the increased resolution maintained, by solving simultaneous linear equations that relate the PSF and the integrated PSF mathematically. The method does not require any increase in the memory or any modification of the simulation program. The proposed method has been examined through simulations by comparing the PSFs derived by the method with those directly generated from the Monte Carlo simulation, and it has been shown to maintain high accuracy. The significant improvement of the spatial resolution achieved for different types of substrate systems indicates that the proposed method is effective and practical.

ACKNOWLEDGMENT

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