## Enhancement of Spatial Resolution in Generating Point Spread Functions by Monte Carlo Simulation in Electron-beam Lithography

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## Abstract

One of the widely-used methods to generate points spread functions (PSF's) in electron-beam lithography is to rely on the Monte Carlo simulation. A substrate system including the resist layer is modeled as a threedimensional (3-D) 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 3-D *PSF* sampled at the interval of cell size. The spatial resolution, i.e., the size of cell, depends on the size of the 3-D array. A higher spatial resolution or a smaller cell requires a larger array. The maximum size of array is determined by the size of memory available on a computer. It is often the case that the desired resolution is not achievable due to the limited memory size, especially on a PC. In this study, a novel method for enhancing the spatial resolution of *PSF* without increasing the size of memory has been developed, based on the mathematical formulation.

Let p[i][j][k] represent the 3-D array or PSF where k corresponds to the resist (substrate) depth dimension. A 3-D PSF may be considered as a stack of two-dimensional (2-D) PSF's where a 2-D PSF is a layer of p[i][j][k] with k fixed, to be denoted by  $p_k[i][j]$ . In the proposed method, in order to increase the spatial resolution in the i dimension, the substrate system is modeled by a 2-D array P[i][k] where the cell is elongated in the j dimension, long enough to cover the electron scattering range, i.e.,  $P[i][k] = \sum_j p[i][j][k]$ . Equivalently,  $P_k[i] = \sum_j p_k[i][j]$  for a fixed k (layer). Since the 2-D PSF is radially symmetric,  $p_k[i][j]$  may be replaced by a 1-D array or PSF,  $p_k[l]$ . Then,  $P_k[i]$  can be expressed, for each i, by a linear equation of the elements in the set  $\{p_k[l] \mid l = 1, 2, \dots\}$  since 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  $P_k[i]$ . The simultaneous linear equations of  $P_k[i]$  are solved for  $p_k[l]$  which is the PSF to be found. Note that the spatial resolution of  $p_k[l]$  is the same as that of  $P_k[i]$ .

The key idea of the proposed method is to reduce the dimensionality in the representation of the simulation space, exploiting the fact that the PSF is radially symmetric, and increase the spatial resolution in the remaining dimension(s). Suppose that p[i][j][k] is of the size  $n \times n \times n$  and P[i][k] of the size  $N \times N$ . If the size of 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 cell) achieved by the proposed method is proportional to  $\frac{1}{N} = \frac{1}{\sqrt[2]{M}}$ , compared to  $\frac{1}{n} = \frac{1}{\sqrt[3]{M}}$  by the conventional method. That is, the spatial resolution is improved  $\sqrt[6]{M}$  times by the proposed method, e.g., 10 times higher resolution when  $M = 10^6$ .

The proposed method has been tested with the data generated from the CASINO software and the results obtained for the substrate system of 300nm PMMA on Si with 50 keV are provided in Figs. 1 and 2. The highest spatial resolution possible on a PC with 2 Gbytes is about 40nm when the substrate system is modeled by a 3-D array (p[i][j][k]). The accuracy of the proposed method has been examined for the spatial resolution of 40nm by comparing the PSF (Fig. 1(b)) derived from  $P_k[i]$  by the method to the PSF (Fig. 1(c)) directly generated from the CASINO software. It is clear that the two PSF's match well, indicating high accuracy of the proposed method. Modeling the substrate system by a 2-D array improves the spatial resolution to about 4nm and the corresponding P[i][k] is shown in Fig. 2(a). The PSF with the spatial resolution of 4nm, derived by the proposed method, is provided in Fig. 2(b). Note that on a PC with 2 Gbytes this high-resolution PSF cannot be generated using the 3-D array p[i][j][k].

The proposed method provides a practical way to enhance the spatial resolution of PSF's generated from the Monte Carlo simulation. In this paper, a detailed description of the proposed method will be presented.



Figure 1: Results for the resist layer with spatial resolution  $\approx 40$ nm: (a)  $P_k[i]$  generated by CASINO, (b)  $PSF(p_k[l])$  derived from  $P_k[i]$  by the proposed method, and (c)  $PSF(p_k[i, j])$  generated by CASINO.



Figure 2: Results for the resist layer with spatial resolution  $\approx 4$ nm: (a)  $P_k[i]$  generated by CASINO and (b)  $PSF(p_k[l])$  derived from  $P_k[i]$  by the proposed method.