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Total process function in electron beam lithography

Karl E. Hoffmann [a,*], Michael Asteiner [b], Peter Speckbacher [b]

[a] University of Applied Sciences Rosenheim, Hochschulstrasse 1, D-83024 Rosenheim, Germany
[b] Dr. Johannes Heidenhain GmbH, Dr.-Johannes-Heidenhain-Strasse 5, D-83301 Traunreut, Germany

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ABSTRACT

Proximity effect correction software in electron beam lithography needs the pattern layout and the total process function (TPF) as an input. This function is determined by electron scattering in resist layer and substrate, the beam blur and diffusion effects during development and post processing. Measuring the TPF is difficult. A three-step method is therefore suggested to calculate the TPF for thin resist layers: Monte Carlo simulation of electron scattering followed by 2d-convolutions with the beam blur and a diffusion function. The convolution algorithm will be described in detail. Experimental data taken from literature are used to verify this calculation method. The method is also useful to assess the quality of the lithographic process.

1. Introduction

To meet future requirements of mask fabrication by electron beam lithography the correction of the proximity effect must be improved. The long-range nature of the proximity effect is due to the scattering of electrons in the resist layer and substrate. Its short-range character is predominantly caused by beam blur and diffusion effects during post processing.

The software used for proximity effect correction (PEC) needs the mask layout and a total process function (TPF) which quantifies the proximity effect as an input. Measuring the proximity effect directly is difficult and time-consuming. We propose a three-step method to calculate the TPF including simple empirical models for beam profile and process effects.

In the first step of the calculation, the point spread function (PSF) is computed by Monte Carlo simulation with the beam diameter set to zero. Subsequently, to include the beam blur, the PSF will be 2d-convoluted with the beam profile. This second step yields the energy deposition function (EDF) which describes the energy deposition in the resist layer due to the electron beam. The influence of all post-exposure process steps are represented by the process function. This function will finally be 2d-convoluted with the EDF to obtain the TPF.

The core of this method is a fast, robust and accurate numerical algorithm for the 2d-convolution. Any function can be used for the beam profile and the process function. But in either case a Gaussian function is most convenient, assuming that no single effect dominates the underlying process.

2. Calculation

2.1. First step – Computing the point spread function

The PSF is calculated for a point beam with the PENELOPE software [1]. In order to describe the energy deposition precisely in the range up to 1 μm, the generation of secondary electrons and plasmon excitations must be explicitly taken into account [2,3]. The result of the simulation is a piecewise constant function (histogram) defined on non-uniform intervals D_j ($j = 1,2,\ldots m$). Let PSF_j be the function value on the interval D_j.

2.2. Second step – 2d-Convolution with beam blur

For a thin resist layer and a perpendicular incident beam with beam blur $B(r)$ the deposited energy in the resist layer is determined by

$$\mathrm{EDF}(\vec{r}) = \iint_{\mathbb{R}^2} B(\vec{r}\,') \,\mathrm{PSF}(|\vec{r}\,' - \vec{r}\,|)\, d\vec{r}\,' \tag{1}$$

Utilizing the rotational symmetry of the problem and changing over to polar coordinates leads to

$$\mathrm{EDF}(r) = 2\int_{R=0}^{\infty} \mathrm{PSF}(R)\left[\int_{\theta=0}^{\pi} B\left(\sqrt{r^2+R^2+2rR\cos\theta}\right)d\theta\right] RdR \tag{2}$$

* Corresponding author. Tel.: +49 8031 805 2417.
E-mail address: karl.hoffmann@fh-rosenheim.de (K.E. Hoffmann).

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where r is the distance from the beam axis.

The outer integration is done by piecewise integration over the subintervals D_j. PSF_j can be factored out of the corresponding integral

$$\mathrm{EDF}(r) = 2\sum_{j=1}^{m} \mathrm{PSF}_j \int_{R\in D_j} \left[\int_{\theta=0}^{\pi} B\left(\sqrt{r^2+R^2+2rR\cos\theta}\right) d\theta \right] R\,dR \tag{3}$$

Let r_i be the center of the interval D_i and $\mathrm{EDF}_i = \mathrm{EDF}(r_i)$, then with

$$B_{ij} = 2\int_{R\in D_j} \left[\int_{\theta=0}^{\pi} B\left(\sqrt{r_i^2+R^2+2r_iR\cos\theta}\right) d\theta \right] R\,dR \tag{4}$$

the convolution will be reduced to a linear transformation

$$\mathrm{EDF}_i = \sum_{j=1}^{m} B_{ij} \cdot \mathrm{PSF}_j \tag{5}$$

The convolution should preserve energy. Energy conservation is therefore a good measure for the numerical quality of the algorithm. The error is typically of the order of 0.001%. For more information, see Supplementary data, Appendix A.1.

Averaging $\mathrm{EDF}(r)$ over D_i

$$\mathrm{EDF}_i = \frac{1}{V_i}\int_{D_i} \mathrm{EDF}(r) 2\pi r\,dr \tag{6}$$

increases the accuracy, where $V_i = 2\pi r_i d(D_i)$ is the volume of the bin corresponding to the interval D_i. The integration can be performed with Newton–Cotes or Gaussian quadrature formulas with few integration points.

For a Gaussian beam profile

$$B(r) = \frac{1}{2\pi\sigma^2}\cdot\exp\left(-\frac{r^2}{2\sigma^2}\right) \quad \text{with FWHM} = 2\sqrt{2\cdot\ln(2)}\sigma \tag{7}$$

the inner integral in (4) can be done analytically.

$$\int_{\theta=0}^{\pi} B\left(\sqrt{r_i^2+R^2+2r_iR\cos\theta}\right) d\theta = \frac{1}{2\pi\sigma^2}\int_{\theta=0}^{\pi} \exp\left(-\frac{r_i^2+R^2+2r_iR\cos\theta}{2\sigma^2}\right) d\theta = \tag{8}$$

$$\frac{1}{2\pi\sigma^2}\cdot\exp\left(-\frac{r_i^2+R^2}{2\sigma^2}\right)\int_{\theta=0}^{\pi}\exp\left(-\frac{r_iR\cos\theta}{\sigma^2}\right)d\theta = \frac{1}{2\sigma^2}\cdot\exp\left(-\frac{r_i^2+R^2}{2\sigma^2}\right)\cdot I_0\left(\frac{r_iR}{\sigma^2}\right) \tag{9}$$

$I_0(z)$ is the modified Bessel function of the first kind with order zero [4]. This function increases exponentially. To avoid arithmetic overflow an asymptotic expansion for $I_0(z)$ is used for large arguments [4].

$$\frac{1}{2\sigma^2}\cdot\exp\left(-\frac{r_i^2+R^2}{2\sigma^2}\right)\cdot I_0\left(\frac{r_iR}{\sigma^2}\right) \simeq \exp\left(-\frac{(r_i-R)^2}{2\sigma^2}\right)\cdot\frac{1+\sigma^2/(8r_iR)}{2\sigma\sqrt{2\pi r_iR}} + \mathcal{O}\left[\left(\frac{r_iR}{\sigma^2}\right)^{-2}\right] \tag{10}$$

2.3. Third step – 2d-Convolution with process function

The EDF will be convoluted with a process function $P(r)$, to include the influence of post-exposure process steps:

$$\mathrm{TPF}(\vec{r}) = \iint_{\mathbb{R}^2} \mathrm{EDF}(\vec{r}')P(|\vec{r}'-\vec{r}|)d\vec{r}' \tag{11}$$

The algorithm from the 2nd step can be reused, since the convolution is a commutative operation.

2.4. Fit procedure

A nonlinear Levenberg–Marquardt algorithm was used for all fits. The loss function

$$\lambda(\sigma) = \sum_{i=1}^{m}[r_i\cdot\mathrm{TPF}_{simulated}(r_i,\sigma) - r_i\cdot\mathrm{TPF}_{measured}(r_i,\sigma)]^2 \tag{12}$$

is suggested by the energy $2\pi r\,\mathrm{TPF}(r)dr$ deposited in a cylinder with radius r.

3. Results and discussion

The experimental data used to evaluate the three-step method are taken from literature. The experimental TPF was fitted to the computed PSF in the range above 1 μm. In this region the short-range effects like beam blur and diffusion do not affect the TPF and the simulated PSF computed during the 1st step should be in good agreement with the measured values. Simulating and matching the PSF both with and without generation of fast secondary electrons helps to specify the fit range (see Supplementary data, Appendix A.2).

All our PENELOPE simulations were carried out with 1 million primary electrons.

3.1. PMMA process without process effects

A PMMA process requires no post-processing steps, diffusion effects are therefore not to be expected. The TPF is only influenced by electron scattering and beam blur. Rishton and Kern [5] measured the TPF for a PMMA resist layer with a thickness of 125 nm both on a solid silicon substrate and on a thin silicon nitride membrane. The energy of the primary electrons was equal to 25 keV and the beam FWHM amounted to 10–20 nm.

The PSF was simulated for the top layer of the resist with a thickness of 25 nm. The density of the deposited energy increases with depth for this experimental setup. The dose to clear for the whole resist layer is therefore achieved, if the dose in the top layer exceeds that value (see Supplementary data, Appendix A.3).

The experimental data for the solid silicon substrate were adjusted to the simulated PSF in the range from 2 to 5 μm (see Fig. 1). Above 0.05 μm the simulated PSF coincides well with the measured TPF. To obtain the EDF a Gaussian beam blur with fit parameter FWHM was convoluted with the PSF. The EDF was fitted to match the experimental data with the best fitting value of 19.6 nm. This result is in agreement with the diameter range stated above.

To prevent electron backscattering, Rishton and Kern [5] replaced the bulk silicon substrate by a 60 nm thick silicon nitride membrane. The PMMA process remained unchanged. To get the EDF for this stack the PSF was recalculated and convoluted with a Gaussian beam with FWHM 19.6 nm. The experimental data were adjusted with the scaling factor which was determined for the solid silicon substrate. The simulated and experimental data are compared in Fig. 2.

The coincidence demonstrates the possibility to extract the characteristic process parameters and to transfer them to another stack.

3.2. ZEP520 process with process effects

The three-step method is suitable for gaining the process function from a measurement of the TPF. This will be demonstrated by