Modeling approaches for electron beam lithography

E Koleva\textsuperscript{1,2}, K Vutova\textsuperscript{1}, B Asparuhova\textsuperscript{1}, I Kostic\textsuperscript{3}, K Cvetkov\textsuperscript{1,2} and V Gerasimov\textsuperscript{1,2}

\textsuperscript{1}Institute of electronics, Bulgarian Academy of Sciences, 72, Tzarigradsko shose, Sofia 1784, Bulgaria
\textsuperscript{2}University of Chemical Technology and Metallurgy – Sofia, 8, Kliment Ohridski blvd., Sofia 1756, Bulgaria
\textsuperscript{3}Institute of Informatics, Slovak Academy of Sciences, Dubravska cesta 9, 845 07 Bratislava, Slovak Republic

e-mail: eligeorg@abv.bg

Abstract. In this paper, a study based on the mathematical modelling, applying different process simulation tools (CASINO, TREM, SELID) for characterization of PMMA resist and for the improvement of the resolution concerning the critical dimensions of nano-patterning by electron beam lithography (EBL) is presented. Data for important EBL characteristics (energy deposition function, proximity effect parameters, solubility rate, etc.) are obtained by applying different approaches (Monte Carlo methods, regression models, etc.).

1. Introduction

Electron beam lithography (EBL) is one of the most popular technological methods in R&D for device prototyping, where there is a need to define and obtain fine patterns. This top-down technique is important for nanofabrication that enables reliable patterning with high resolution (down to the nm scale) for production of many devices such as nanowires, quantum devises, high-frequency electronics, etc. [1]. This method is based on the physical-chemical changes in the resist layer and commonly used resists are polymers that are dissolved in a liquid solvent in order to enhance the lithography performance of the material. The main advantages of the widely used positive tone PMMA (polymethyl-methacrylate) resist, which has important applications in nanolithography, are ultimate resolution (less than 10 nm), high contrast, good adhesion to most substrates, etc.

In many computer codes the penetration of irradiating electrons in the polymer layer is calculated utilizing Monte Carlo method [2, 3, 4]. At electron beam lithography, the electron scattering is modeled by using a point spread function (PSF), which shows how much energy is distributed throughout the resist when a single point is exposed. In this way the energy of the penetrating electrons and the deposited energy losses in a small local region of the sample are assessed. The point exposure energy deposition function (EDF) [2, 5, 6, 7] is calculated by estimation of the energy distribution along the resist when a single point is exposed. It is determined as a histogram function depending on the radial distance from the direction of the electron penetration and on the depth of resist layer. Often this function is called also proximity function because it determines the proximity effect.

CASINO is a software for simulation of the electron movement trajectories, the distribution of the backscattered and the absorbed in the sample energies during electron beam exposure. The software...
uses a single-scattering algorithm for modeling low-energy beam interactions in bulk and thin foil samples.

The program offers a user-friendly graphical user interface such that the specific conditions for the simulation of the exposure process during electron beam lithography can be easily set.

In this paper an exposure and development study of Poly-methyl methacrylate resist with 800-1800 nm thickness on Si substrate is presented. The electron energy is 30 keV. The absorbed energy is simulated by the CASINO software and by our simulation tool TREM [2]. The process of resist development was performed in the program SELID. Results concerning the estimated dissolution rate, based on obtained experimental data are also presented.

2. Electron beam exposure

Electron beam lithography experiments on Poly-methyl methacrylate (PMMA) resist with structural formula \((C_5H_8O_2)_n\) were made. It is one of the first materials used in electron beam lithography as a resist. It is a standard positive resist and it has one of the highest resolutions. The electron energy was 30 keV. Electron beam with Gaussian distribution and a diameter of 10 nm was applied. Silicon (Si) was chosen for a substrate.

The CASINO program applies the Monte Carlo method, which simulates the electron trajectories by generating random numbers. When calculating, it is assumed that the diffusing atom is represented by Rutherford’s shielded potential, and the deviation of the trajectory of the penetrating electron at impact is obtained from the differential section of the elastic scattering. The energy losses experienced by the penetrating electron along its entire trajectory until it is stopped or left out of the sample is calculated on the BETt’s score for inelastic losses from the penetrating electron strikes with the electrons of the sample.

The electron trajectories are calculated using the following formulas [8]:

\[
X_0 = \frac{d \log(R_1)}{2 \times 1.65} x \cos(2\pi R_2) \tag{1}
\]

\[
Y_0 = \frac{d \log(R_1)}{2 \times 1.65} y \cos(2\pi R_3) \tag{2}
\]

\[
L = -\lambda_{el} \log(R_4) \tag{3}
\]

\[
\frac{1}{\lambda_{el}} = \rho N_0 \sum_{i=1}^{n} \frac{c_i \sigma_{el}^i}{A_i} \tag{4}
\]

\(R_i\) are random numbers uniformly distributed between 0 and 1, \(d\) is the electron beam diameter.

The distance \(L\) [nm] between two successive collisions is [8]:

\[
L = -\lambda_{el} \log(R_4)
\]

\[
\frac{1}{\lambda_{el}} = \rho N_0 \sum_{i=1}^{n} \frac{c_i \sigma_{el}^i}{A_i}
\]

\(C_i, A_i\) are the weight fraction and atomic weight of element \(i\), respectively, \(\rho\) is the density of the region (g/cm\(^3\)) and \(N_0\) is the Avogadro’s constant.

![Figure 1. Simulated electron trajectories.](image-url)
A simulation with 15,000 electron trajectories was performed. After the simulation, the software provides a series of graphs showing different process data. 200 from the simulated 15,000 by CASINO electrons trajectories are given in figure 1: in blue color are shown the trajectories of the transmitted electrons, and in red - the backscattered electron trajectories.

Figure 2 presents the distribution of the absorbed energy in the sample in radial direction x and in resist depth z for electron beam energy of 30 keV in 1300 nm PMMA resist on Si. In figure 3 the maximum penetration depth of the electrons in the sample, as hits, normalized by the number of primary simulated electrons is presented.

Figure 4 shows graphically the dependence of the absorbed electron energy on the radial distance (from the direction of the initial movement of the electron beam) at the resist/substrate interface, obtained using TREM simulation Monte Carlo tool, developed in the IE-BAS [2].

In figures 5–6, the simulated by the CASINO software results, connected with the backscattered electrons, are shown. Figure 5 presents the maximum penetration depth of electron trajectories in the sample that will escape the sample surface and figure 6 presents the energy of backscattered electrons when escaping the surface of the sample.

**Figure 2.** Distribution of the absorbed energy in the sample on x and z axes in PMMA resist at electron beam energy 30 keV. Number of electron trajectories simulated is 15,000.

**Figure 3.** Maximum penetration depth in the sample of the electron trajectories.

**Figure 4.** Absorbed electron energy vs. the radial distance (from the direction of the initial movement of the electron beam).
3. Proximity effect

The particle scattering causes the energy deposition at any point to differ from the desired energy distribution, needed for the exposed pattern configuration management. The absorbed energy at any point can be calculated by summing the energy loss during the irradiation of the resist points, lying in the region of several μm. This phenomenon is known as proximity effect (PE) by the configuration change of the exposed pattern and/or by the dose distribution. Thus the particle scattering or the proximity effect limits the pattern resolution and the distance between the adjacent-situated structures. Unwanted energy deposition occurs in unexposed regions, which leads to undesirable deformations of the developed profiles. The development process also influences the quantitative deformation characteristics of the microstructure connected to the proximity effect.

An approximation of the absorbed energy distribution, valid for the Si substrate, is a sum of two Gaussian functions (“proximity function”):

$$f(r) = k \left[ \exp \left( -\frac{r^2}{\delta_f^2} \right) + \eta_E \cdot \frac{\delta_b^2}{\delta_f^2} \cdot \exp \left( -\frac{r^2}{\delta_b^2} \right) \right]$$

where $k$ – a constant, $\delta_f$ and $\delta_b$ – characteristic widths of the forward and the backward scattering particles, $\eta_E$ is a measure of the backscattering over forward scattering contribution ratio of the absorbed energy.

The changes in the values of the PE parameters along the depth of the resist ($z$, or in coded values $x$) were calculated using an original Monte Carlo technique [2] for different PMMA resist thicknesses – 800 nm, 1300 nm and 1800 nm. The input data was the 2D arrays containing the discrete EDF obtained as a result of the trajectory modeling by TREM. The estimated models for each resist thickness for the parameters $\eta_E$, $\delta_f$ and $\delta_b$ are presented in table 1.

In table 2 are presented the assumed denotations for the parameter depth in the resist, depending on the PMMA resist thickness.

The conversion from natural ($z_i$) to dimensionless coded ($x_i$) values and vice versa can be done by the formula:

$$x_i = \frac{2z_i - (z_{max,i} + z_{min,i})}{z_{max,i} - z_{min,i}}.$$

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**Figure 5.** Maximum penetration depth in the sample of electron trajectories that will escape the sample surface.

**Figure 6.** Energy of backscattered electrons when escaping the surface of the sample.
The depth in the resist. For the estimation of the PE parameters for any resist thicknesses in the region 800-1800 nm it is more convenient to use overall regression models for each of the considered parameters - \( \eta_f \), \( \delta_f \) and \( \delta_b \). Their dependence on two factors is taken into account – the depth in the resist \((z_t, \text{nm} / x_t, \text{table 3})\) and the resist thickness \((z_s, \text{nm} / x_s)\). The estimated generalized regression models are presented in table 4. The accuracy of the models takes into consideration the prediction properties over the whole region of the variation of the chosen factors, but it should be kept in mind that the regions are constrained by the possible depth of the resist under specified resist thickness. In figure 7 contour plots of the dependencies of the PE parameters \( \eta_f \) (a measure of the backscattering over forward scattering contribution ratio of the absorbed energy), \( \delta_f \) and \( \delta_b \) (the characteristic widths of the forward and the backward scattering particles) on the depth in the resist and the resist thickness are presented. The colored areas are the zones where the values of the depth in the resist are not available.

| Resist | PE parameter | Regression model | R², % |
|--------|--------------|------------------|------|
| thickness |             |                  |      |
| 800 nm  | \( \eta_f \) | \( \hat{y}_1(x_1) = 0.22647259 + 0.06764457x_1 + 0.34278528x_1^4 \) | 96.065 |
|         | \( \delta_f, \text{\mu m} \) | \( \hat{y}_2(x_1) = 0.05324728 + 0.0022172x_1 - 0.00141404x_1^2 \) + 0.03074833x_1^4 | 99.841 |
|         | \( \delta_b, \text{\mu m} \) | \( \hat{y}_3(x_1) = 2.8204608 + 1.8172518x_1^2 + 0.11464655x_1^3 \) - 1.9545286x_1^4 | 93.845 |
| 1300 nm | \( \eta_f \) | \( \hat{y}_4(x_2) = 0.42036949 + 0.17858961x_2 - 0.31902275x_2^2 \) + 0.15298222x_2^4 | 99.948 |
|         | \( \delta_f, \text{\mu m} \) | \( \hat{y}_5(x_2) = 0.0669447 + 0.01476891x_2 - 0.03022446x_2^2 \) - 0.01767763x_2^3 | 96.326 |
|         | \( \delta_b, \text{\mu m} \) | \( \hat{y}_6(x_2) = 2.9709817 - 0.60599526x_2 + 0.11678104x_2^2 \) + 0.56021804x_2^3 | 98.319 |
| 1800 nm | \( \eta_f \) | \( \hat{y}_7(x_3) = 0.30975127 + 0.28909426x_3 - 0.24156188x_3^3 \) + 0.32462558x_3^4 | 96.992 |
|         | \( \delta_f, \text{\mu m} \) | \( \hat{y}_8(x_3) = 0.08783351 + 0.00472963x_3 - 0.20287343x_3^2 \) + 0.13914999x_3^4 | 95.316 |
|         | \( \delta_b, \text{\mu m} \) | \( \hat{y}_9(x_3) = 3.2583843 + 0.33558813x_3 - 0.27148222x_3^2 \) - 0.74921x_3^3 | 99.865 |

| Resist thickness | Depth in the resist | Coded | Lower level \((z_{\text{min},i})\) | Upper level \((z_{\text{max},i})\) |
|------------------|----------------------|-------|-------------------------------|-----------------|
| 800 nm           | \( z_1 \)           | \( x_1 \) | 20                            | 800             |
| 1300 nm          | \( z_2 \)           | \( x_2 \) | 30                            | 1290            |
| 1800 nm          | \( z_3 \)           | \( x_3 \) | 40                            | 1800            |

Table 3. Overall factors.

| Factor                      | Dimension | Coded | Lower level \((z_{\text{min},i})\) | Upper level \((z_{\text{max},i})\) |
|-----------------------------|-----------|-------|-------------------------------|-----------------|
| Depth in the resist - \( z_4 \) | nm        | \( x_4 \) | 20                            | 1800             |
| Resist thickness - \( z_5 \)   | nm        | \( x_5 \) | 800                            | 1800             |
Table 4. Overall regression models.

| PE parameter | Regression model | R  |
|--------------|------------------|----|
| $\eta_E$     | $\hat{\eta}_1(x_4, x_5) = 0.39970417 + 0.29203616x_4 - 0.12255184x_5 + 0.3547082x_4x_5^2 - 0.22531466x_4x_5^3$ | 0.81 |
| $\delta_f$, nm | $\hat{\delta}_1(x_4, x_5) = 67.612478 - 21.001033x_4 - 48.189135x_4^2 + 22.487086x_4x_5^2$ | 0.84 |
| $\delta_b$, nm | $\hat{\delta}_2(x_4, x_5) = 3025.3192 - 105.90543x_4 + 91.149872x_5 - 298.74041x_4x_5$ | 0.73 |

Figure 7. Contour plots of PE parameters a) $\eta_E$, b) $\delta_f$ and c) $\delta_b$ as a function of the depth in the resist – $z_4$ and PMMA resist thicknesses – $z_5$.

4. Resist profile development

The development of PMMA is realized by selectively dissolving the irradiated and truncated polymer chains. The rate of dissolution depends on the exposure dose and the chemical characteristics of the developer. Figure 8 and figure 9 present correspondingly the experimentally measured contrast curves and the estimated dissolution rates for PMMA. The influence of different developers (MIBK:IPA 1:3 and H2O:IPA 3:7) and resist thickness were considered. The obtained dose to clear for PMMA with
thickness $T_0 = 1165$ nm, applying developer MIBK:IPA 1:3 and development time 60 seconds was $D_0 = 182 \, \mu C/cm^2$.

Figure 8. Contrast curves for PMMA on Si:
curve 1 - $T_0 = 300$ nm, developer H$_2$O:IPA 3:7, dose to clear $D_0 = 122 \, \mu C/cm^2$;
curve 2 - $T_0 = 1134$ nm, developer H$_2$O:IPA 3:7, $D_0 = 147 \, \mu C/cm^2$;
curve 3 - $T_0 = 300$ nm; developer MIBK:IPA 1:3, $D_0 = 157 \, \mu C/cm^2$;
curve 4 - $T_0 = 1165$ nm, developer MIBK:IPA 1:3, $D_0 = 182 \, \mu C/cm^2$.

Figure 9. Dissolution rate dependence for:
curve 1 - $T_0 = 1165$ nm, developer MIBK:IPA 1:3, $D_0 = 182 \, \mu C/cm^2$
curve 2 - $T_0 = 1134$ nm, developer H$_2$O:IPA 3:7, $D_0 = 147 \, \mu C/cm^2$.

SELID (Simulation of Electron Beam Lithography in 2 and 3 Dimensions) provides a comprehensive simulation tool covering most aspects of today's advanced electron beam lithography, such as process optimization and parameter determination for the electron beam proximity effect correction.

The code SELID measures three developed line profile widths. First is the width of the developed profile, measured at the bottom at the interface between the resist and the substrate surface called width at the substrate. The width at a height of 5% of the initial resist thickness $d_0 (0.05d_0)$ from the substrate called width at the bottom is measured too. In the output data there is also the width at the top of resist profile determined at 90% of the initial resist thickness.

Another output value is the thickness loss of the developed resist profile – in percent with respect to the nominal resist thickness.

In figure 10 the simulated PMMA resist profile after exposure with electron energy 30 keV and development with MIBK:IPA 1:3 for 360 sec is presented and the proximity effect can be seen. The obtained geometry parameters are: width at the substrate – 0.535 \, \mu m, width at the bottom 0.709 \, \mu m, width at the top – 0.467 \, \mu m, the average sidewall angle – 96.88°, thickness loss – 5.5%.
5. Conclusions
In this paper, important process characteristics such as energy deposition function, proximity effect parameters, solubility rate are calculated and estimated and developed profiles in PMMA resist are simulated for different e-beam lithography conditions (resist thickness, used developers). Results obtained by mathematical modeling and lithography processes (exposure and development) simulation applying different tools (CASINO, TREM, SELID) for characterization of PMMA resist in order to improve the resolution at electron beam lithography are presented. The electron beam lithography process is essential for the construction of small-scale electronic components. Real-time experiments take a long time and resources, they are conducted only in specialized laboratories, require highly skilled staff and optimization of process parameters in real conditions is an extremely difficult and labor-intensive task. Software products such as SELID, CASINO and TREM provide a virtual environment for learning the process and conducting experiments even by less knowledgeable professionals, they provide a good opportunity to explore the impact of parameters such as accelerating voltage, number of electrons, exposure dose, thickness and structure of the resist, developer and others.

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References
[1] Mohammad M, Muhammad M, Dew S and Stepanova M 2012 Fundamentals of Electron Beam Exposure and Development, (Springer-Verlag, Wien), chapter 2 p 11
[2] Vutova K and Mladenov G 2010 Lithography ed M Wang (INTECH, Vukovar) chapter 17 pp 319-350
[3] Urbánek M, Kolařík V, Krátký S, Matějka M, Horáček M and Chlumská J 2013 Proc. Int. conf NANOCON 16. - 18. 10. 2013 (Brno: Czech Republic EU)
[4] Indykiewicz K, Paszkiewicz B and Paszkiewicz R 2018 Advance in electrical and electronic engineering 16(2) 246
[5] Lee S-Y, Dai Q, Lee S-H., Kim B-G and Cho H-K 2011 J Vac. Sci. Technol. B Microelectronics and Nanometer Structures 29(6) Nov_Dec 06F902-1 - 06F902-7
[6] Andok R, Bencurova A, Vutova K, Koleva E, Nemec P, Hrkut P, Kostic I and Mladenov G 2016 Journal of Physics: Conference Series 700(1) art no 012030
[7] Mladenov G 2009 Electron and ion technologies (Prof Marin Drinov)
[8] Drouin D, Couture A R, Joly D, Tastet X, Aimez V and Gauvin R 2007 Scanning 29 3