Effects of model polymer chain architectures of photo-resists on line-edge-roughness. Monte Carlo simulations

G P Patsis, and E Gogolides

Institute of Microelectronics (IMEL), NCSR “Demokritos”, P.O. Box 60228, Aghia Paraskevi, Attiki, Greece 15310. Tel: +30 210 6503267, Fax: +30 210 6511723, E-mail: gpatsis@imel.demokritos.gr

Abstract. Sub-100nm device fabrication rules require extremely tight control of line-edge roughness (LER) of patterned structures. During lithographic processes the resist film introduces an initial LER due to its chemical structure and processing. This initial LER evolves during the subsequent processing steps. In order to reduce LER the relation between polymer chain geometrical characteristics and finally measured LER has to be determined. Following this approach three model polymer chain architectures were considered and their LER was determined. A direct relation is seen between the measured LER and the excluded volume constraints on the polymer chain.

1. Introduction

Material roughness plays a predominant role in the fabrication of devices in the sub-100nm range. The understanding of its origins and of the way processes modify its magnitude is essential. Roughness is defined as surface roughness (SR) and line-edge roughness (LER) of fabricated structures. LER is quantified by its sigma value, i.e. the root-mean square (RMS) of the edge position fluctuations. The effect of the lithographic processes (exposure, acid-diffusion, deprotection/cross-linking, and development) is to modulate the inherent resist material roughness and therefore to affect greatly the measured values of LER. Previous work by our group resulted in establishing some understanding of the statistical characteristics of roughness [1-6]. Recent work tried to probe through Monte Carlo simulations the material origins of roughness and the way lithographic processes affect it [7].

Molecular simulations are becoming necessary at the length scales of nanolithography, since material models used for the bulk are no longer applicable. At the same time film thickness of materials used throughout the lithographic steps in modern device fabrication reduce down to the order of tens of polymer chain radiiuses of gyration, resulting in great proportions of surface and line-edge roughness over the total film thickness and width respectively. The dissolution mechanism of these materials is still lacking a final description in the level of full microscopic details. The dissolution of a general positive tone chemically amplified resist film is simulated, using the critical ionization model [8].

The purpose of the current work is to model the effects of polymer chain architecture on an orthogonal lattice, and determine the way the possible chain conformations and packaging, affects the roughness characteristics of the film. Specifically, the polymer film is considered as polymer chains comprising...
random-walks forming linear chains (case I), self-avoiding random-walks forming grafted chains (case II), and self-avoiding random walks forming linear chains (case III). The objective is to relate the geometrical characteristics of the chains (i.e. end-to-end distance and radius of gyration) to the film line-edge roughness of the developed resist lines.

2. Model Description

A stochastic dissolution simulator was built based on the critical ionization fraction [7]. Its basic advantage is its high speed in the determination of the final edge profile. In a single dissolution circle it determines the chains that have deprotection fraction greater or equal to the critical ionization fraction and removes them from the lattice, revealing the resist side surface at once. Details about the dissolution algorithm can be found in [8]. Its 2D version is utilized in this article to calculate the LER of resist edges, 256nm in height, and under ideal exposure conditions, i.e. with aerial image contrast equal to 1.

Case-I of polymer chains considered in this work, can grow in any lattice direction, can cross other chains and even can retrace their own path (Figure 1(a)). This is the case of a random walk (RW). We use the term “full sharing” to describe the fact that during chain insertion, the generated monomer sites can accommodate more than one monomer which belong to different chains without checking for excluded volume constraints. Therefore, as “site-sharing” is described the case where a lattice site accommodates more than one monomer. Case-II of chain insertion is the randomly grafted polymer chain, shown in figure 1(b). Each monomer is inserted adjacent to a randomly selected one of the previously inserted monomers. Excluded volume effects are taken into account in this case. Necessary sharing is introduced meaning that a site is multiply shared if there are no other possibilities for monomer insertion in a neighboring empty site. An example of a Case-III chain is shown in figure 1(c). Now the chain is linear self-avoiding walk and grows only from one end.

![Figure 1](image-url)

**Figure 1.** (a) Case-I. Random walk chain model. The numbers on monomers indicated the way the chain grows. Double numbers on shaded monomers indicate the sites where more than one monomer is accommodated. (b) A Case-II chain. A randomly grafted polymer. (c) A Case-III chain a linear self-avoiding walk. Case II and III incorporate the notion of necessary site sharing.

3. Results

Figure 2 (a) presents the general view of the 2D simulation lattice. Ideal square pulse exposure is assumed, which totally deprotects the polymer chains on the right side of the lattice from 50nm to 256nm. After application of the dissolution algorithm [10], the monomer fraction shown in figure 2(b) determines the average critical dimension of the structure edge. It is seen that case-III chains (high excluded volume constraints) result accuracy loss in edge position. Figure 2(c) shows the edge coordinates after dissolution...
for the three chain insertion methods. LER and average edge position are the RMS and average obtained from such edge profiles. The final values for these two quantities reported in the following, are from averaging the calculated ones over 100 such profiles.

**Figure 2.** (a) Two dimensional lattice representation. It is filled in each case up to 10% free volume. Polymerization length follows a Poisson distribution. (b) Monomer fraction vs. edge position coordinate. Slope marks the pattern edge (c). Edge profiles.

**Figure 3.** (a) $R_g$, and (b) $R_{ee}$ distribution for the three chain architectures and for two polymerization lengths. (c). Relation of average $R_g$ vs. the chain architecture. Monomer radius is assumed to be 1nm. Otherwise all the values in nm should be multiplied by the appropriate conversion factor.

The distribution of the radius of gyration $R_g$ and end-to-end distance $R_{ee}$ of the polymer chains in the lattice are shown in figure 3(a) and 3(b) respectively, for the $<L>=20$ case. $R_{ee}$ is the distance between the first and last inserted monomer, while $R_g$ is the average distance of all the monomers in a chain from their common center of gravity. Due to the higher magnitude of the excluded volume constraints, case III chains are characterized by higher average values and wider distributions of $R_{ee}$ and $R_g$. These distributions become wider and the corresponding average values increase with polymerization length. The average $R_g$ is seen in figure 3(c). Case I is not physically realizable chain architecture, since no excluded volume constraints are present between the chains. Case II chains incorporate the exclude
volume effects and are characterized by lower average $R_g$ than case III chains. This is attributed to their growth process (their monomer stay closer to each other, more compact and symmetric architecture).

Finally, quantification of LER and edge position is presented in figure 4. The corresponding simulations assumed that in the exposed part of the chain-lattice all monomers became deprotected.

Therefore the effects of acid diffusion characterizing chemically amplified resists are left outside in this study. As is seen in figure 4(a), excluded volume constraints increase LER. Additionally, LER increases with increasing polymerization length. In fact the increase of LER with polymerization length follows the corresponding increase of the radius of gyration of the chains. The edge position control worsens with increased excluded volume, and increase of polymerization length, as is seen quantitatively in figure 4(b). This was already observed qualitatively in figure 3(b) and (c).

![Figure 4](image)

Figure 4. (a) LER variation among the three models of polymer chains for two cases of average polymerization length, $<L>$=10, 20. (b) The corresponding effects on the edge position.

4. Conclusions
The simulation of the effect of model polymer chains on the resist film line-edge-roughness was investigated. For low LER and tight critical dimension control applications, small radius of gyration chains, with limited excluded volume effects, (tightly packed chains) are desired.

5. Acknowledgements
Financial support from European project “More Moore”, and INTEL is kindly acknowledged.

6. References
[1] Patsis G P, Constantoudis V, Tserepi A, Gogolides E, Grozev G and Hoffmann T, Microelec. Engineering 2003 67-68 319
[2] Patsis G P, Constantoudis V, Tserepi A, Gogolides E, and Grozev G 2003 J. Vac. Sci. Technol. B 21 1008
[3] Patsis G P, Tserepi A, and Gogolides E 2003 J. Vac. Sci. Technol. B 21 1019
[4] Eder-Kapl S, Loeschner H, Zeininger M, Kirch O, Patsis G P, Constantoudis V, and Gogolides E, Microelec. Engin. 2004 73-74 252
[5] Constantoudis V, Patsis G P, and Gogolides E 2004 J. Microlithogr. Microfab., Microsyst. 3 429
[6] Constantoudis V, Patsis G P, Leunissen L H A, and Gogolides E 2004 J. Vac. Sci. Technol. B 22 1974
[7] Patsis G P, Constantoudis V, and Gogolides E 2004 Microelec. Engin. 75(3) 297
[8] Tsiartas P C, Flanagan L W, Henderson C L, Hinsberg W D, Sanchez I C, Bonnecaze R T, and Willson C G 1997 Macromolecules 30 4656