Simulator for electron beam lithography (EBL) of nanostructures

M. Stepanova^{1,2}, T. Fito^{1,2}, Zs. Szabó^{1,2}, K. Alti^{1,2}, A.P. Adeyenuwo¹, K. Koshelev^{1,2}, M. Aktary³, and S.K. Dew¹

¹Department of Electrical and Computer Engineering, University of Alberta ²National Institute for Nanotechnology NRC, Edmonton, Alberta ³Applied Nanotools Inc., Edmonton, Alberta

We report a simulator that we developed for analysis and visualization of electron beam exposure, fragmentation, and development of exposed EBL resist, PMMA. Optimizing fabrication of 5-50 nm structures on solid substrates is the target purpose of the simulator. It employs our original suite of kinetic models for transport of electrons in the resist, scission of the polymer chains, and dissolution of the exposed resist in a developer [1-3], see also Fig. 1. The simulator is functional for exposure energies from 1 keV to 30 keV with arbitrary pattern geometries, including fragments of periodic and large pattens with the backscatterning proximity effect included. In the model of exposure, we firstly compute 3D distributions of the probability of main-chain scission [1], which differs from the standard approaches that map energy deposition. Next, we convert the local probability of scission into the local volume fractions of PMMA fragments of various size $F_n(x,y,z)$, where n is the number of monomers in a fragment. The kinetic process of development is described by the movement of the resist-developer interface. We define the rate of dissolution by v = dL/dt, where L(x,y,z,t) is the local depth of shrinking of the resist. The local kinetics of dissolution may be represented by $dL/dt = \langle \eta D_n/L \rangle$, where η is a coefficient that depends on the interaction of developer with PMMA, $D_n(x,y,z)$ is the diffusivity of PMMA fragments of size n, and the averaging is done over the local distribution of the fragments' sizes [3]. This model implies that at the nanoscale, the rate of resist dissolution is a function of the entire history of the process of development, and thus depends on time explicitly. This is different from most available models for EBL resist clearance, which assume a stationary regime with a constant rate of shrinking. Our EBL simulator allows computing detailed 3D distributions of the probability of main chain scission in PMMA for various conditions of exposure, the corresponding volume fractions of small fragmens $n < n_{max}$, where n_{max} can be varied by user, as well as the clearance profiles as functions of development time, as illustrated by Figs. 2-4. In this work we report our numerical study of the exposure and development trends when fabricating 10-30 nm sized objects using 3keV-30 keV exposures, and compare the numeric results with experimental SEM images of nanoscale morphologies in PMMA.

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Fig. 1. Outline of models employed in the simulator for resist exposure and development.



Fig. 2. 3D distribution of the probability of chain scission per monomer in PMMA exposed with 10 keV electrons, for nanostructure composed of four lines of 100 nm in length, and separated by 60 nm. The sizes in the figure are in angstroms.



Fig. 3. The distribution of PMMA fragments with sizes less than 10 monomers, in a periodic grating written with 10 keV electrons.



Fig.4. Clearance profile in a periodic grating written with 3 keV electrons. Red indicates remaining PMMA and blue indicates clearance.