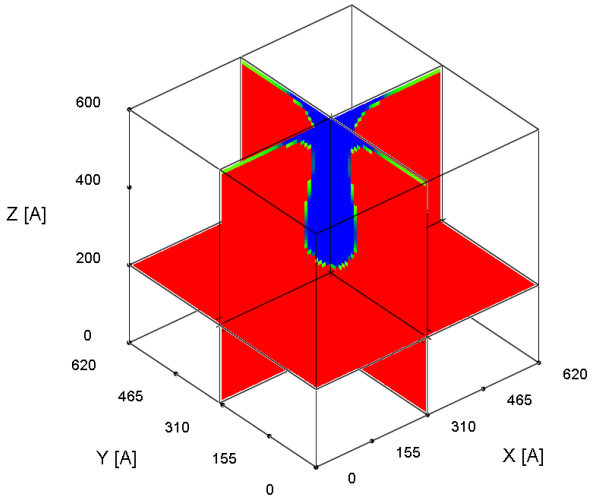
National Institute for Nanotechnology NRC and the University of Alberta
Edmonton, Alberta, Canada

Electron Beam Lithography Simulator

Manual



Annotation

The EBL Simulator is a novel tool for prediction, visualization and analysis of electron beam lithography of structures sized from a few nanometers to micro-scale. The simulator provides 3D predictions, with a 1 nm resolution, for e-beam exposure (1 keV-100 keV voltages), fragmentation, and development profiles for positive tone resists PMMA and ZEP. Individual nanoscale structures, periodic arrays, and parts of large writing patterns of arbitrary geometry are handled with full accounting for forward and backscattering of electrons, as well as for secondary electrons generation. The conditions of development, such as duration and temperature, can also be varied. A user-friendly graphical interface allows for an easy usage of the Simulator. The present manual describes examples of the usage of selected computation and visualization tools of the Simulator.

Contents

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I. Getting Started:
Examples for Low-kV Exposures and Cold Development

Here examples are given of **the usage of basic interface tools** and **simulations of EBL exposure and development**. The examples address thin layers of PMMA resist (40-55 nm) on a Si substrate, exposed with voltages of 1, 3, and 10 keV, and developed in a 1:3 MIBK:IPA mixture at a decreased temperature of –15°C. The pattern is a periodic grating with a 70 nm pitch.

1. Simulation of Exposure

1.1 Launch the **EBL Simulator** from its installed location or programs menu.

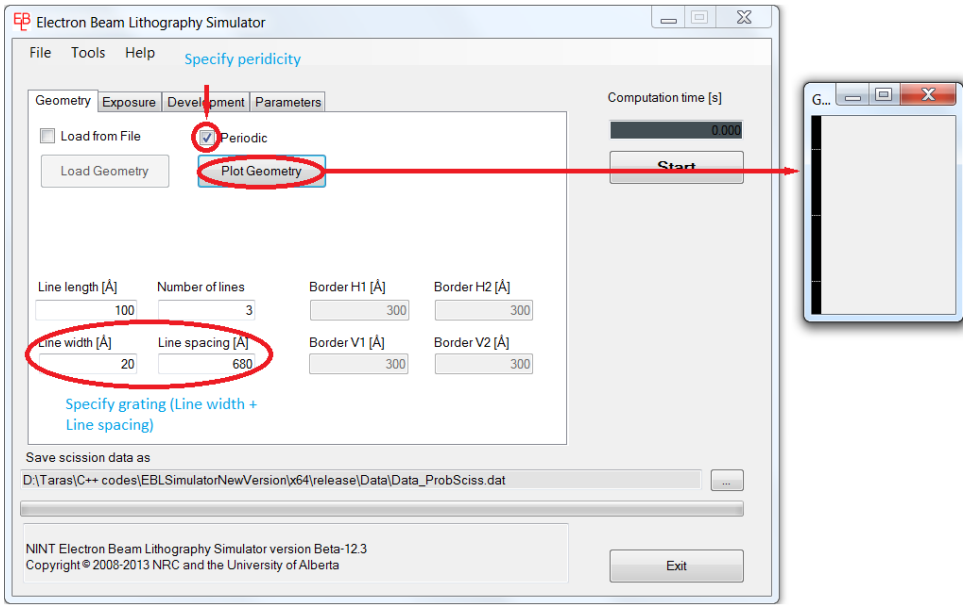

Figure 1: Main window of EBL Simulator: Geometry tab.

Figure 1 shows the main window of the simulator's interface. In the **Geometry** tab you can specify the exposure pattern. If it is desired to simulate a periodic grating, check **Periodic** checkbox. The **Line length** and **Number of lines** can be changed as desired. For the present example, the default values are used. The grating pitch is set by entering the **Line width** and **Line spacing** which defaults to 70 nm. The input pattern can be visualized by clicking the **Plot geometry** button. A window will appear presenting the pattern as shown in the inset in Figure 1.

Note 1.1: The simulator also allows for working with arbitrary periodic patterns other than gratings.

To enter the resist and exposure parameters, select the **Exposure** tab. To run the example shown in Figure 2, enter 1000 eV for the **Exposure energy**, 400 Å for the **Resist thickness**, and 150 pC/cm for the **Line dose**. Then select **PMMA** from the **Resist** dropdown menu. Clicking the **Start** button will run the simulator to generate the yield (probability) of scission data (Figure 3).

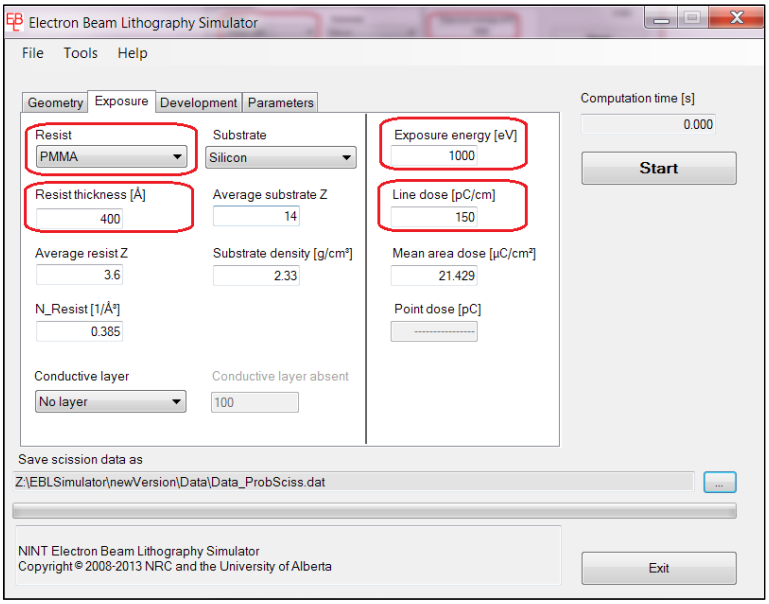

Figure 2: Main window of the EBL Simulator: Exposure tab.

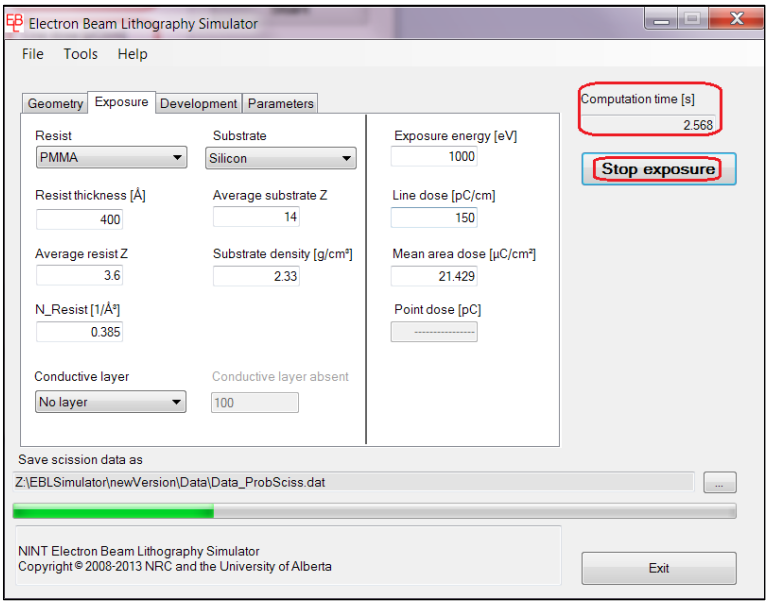

Figure 3: Simulation in progress.

Note 1.2: The yield (or probability) of scissions is equal to the average number of resist main-chain scissions per monomer. The scission yield is computed directly through the differential cross-section for inelastic collisions[1,2]. This approach avoids uncertainties related with the mapping and conversion of distributions of deposited energy.

Note 1.3: A monomer is defined as a nominal unit containing two main chain C-C atoms in a resist. In PMMA, this corresponds to an MMA monomer. In ZEP, a nominal monomer represents averaged properties of two fragment formulations[2].

[1] M. Aktary, M. Stepanova, and S.K. Dew, J. Vac. Sci. & Technol. B, 24 (2006) 768.

[2] K. Koshelev, M.A. Mohammad, T. Fito, K.L. Westra, S.K. Dew, and M. Stepanova, J. Vac. Sci. Technol. B 29 (2011) 06F306.

1.2 Time taken to run the simulation is displayed in the **Computation time** box. The computation can be aborted at any time by clicking the **Stop exposure** button as shown in Figure 3.

1.3 To visualize results of the computation, click **Tools** and select **Plot** as shown in Figure 4. This opens the EBL Simulator Plotting window (Figure 5).

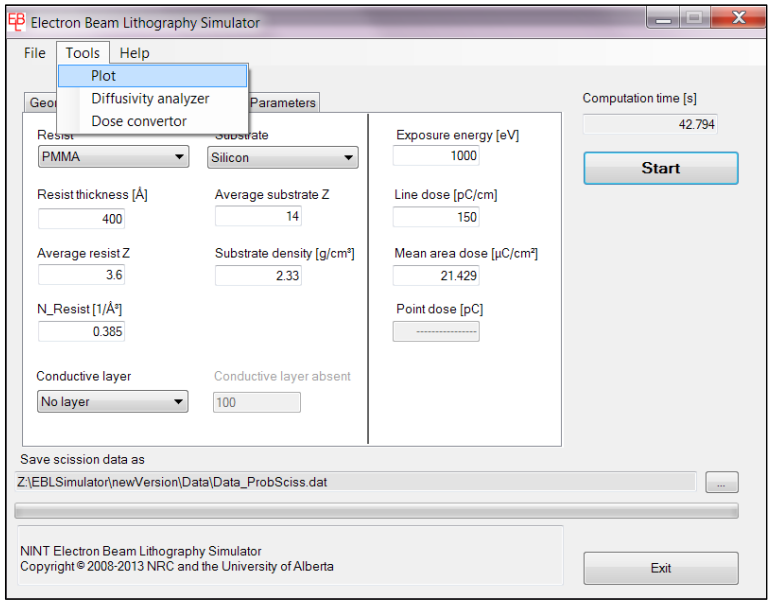

Figure 4: Visualization of simulation results.

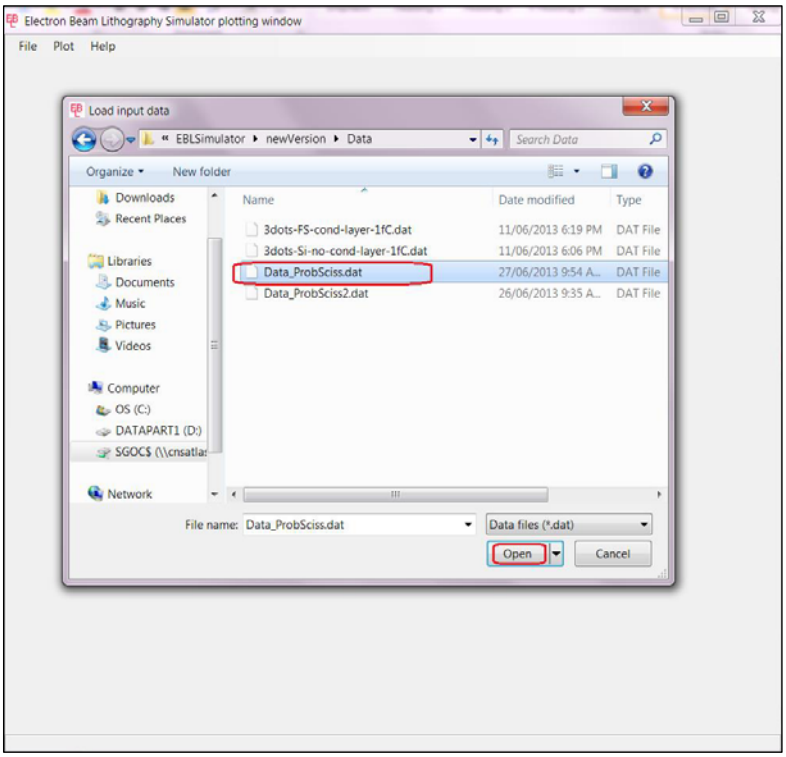

Figure 5: Opening the Probability of Scission file.

1.4 Next, click **File/Open** and select **Data_ProbSciss** file stored in the Data directory as shown in Figure 5. For convenience this file can be renamed in Windows, for example **Data_ProbSciss_1kV_40nm_150pC**.

1.5 3D plot of the simulated yield of scission is displayed in the plotting window in Figure 6. The 3D plot can be rotated, zoomed, translated and analyzed at any location in X, Y and Z directions using the array of buttons highlighted on the right and bottom parts of the window.

1.6 2D Plots of the computed yield of scission can be visualized in 3 directions: XY (top-down), XZ and YZ (sideways). To visualize 2D Plot of the yield of scission, click **Plot/Plot 2D/Plot XZ** as shown in Figure 6. Other 2D Plot visualization options in XY and YZ planes can also be selected if so required.

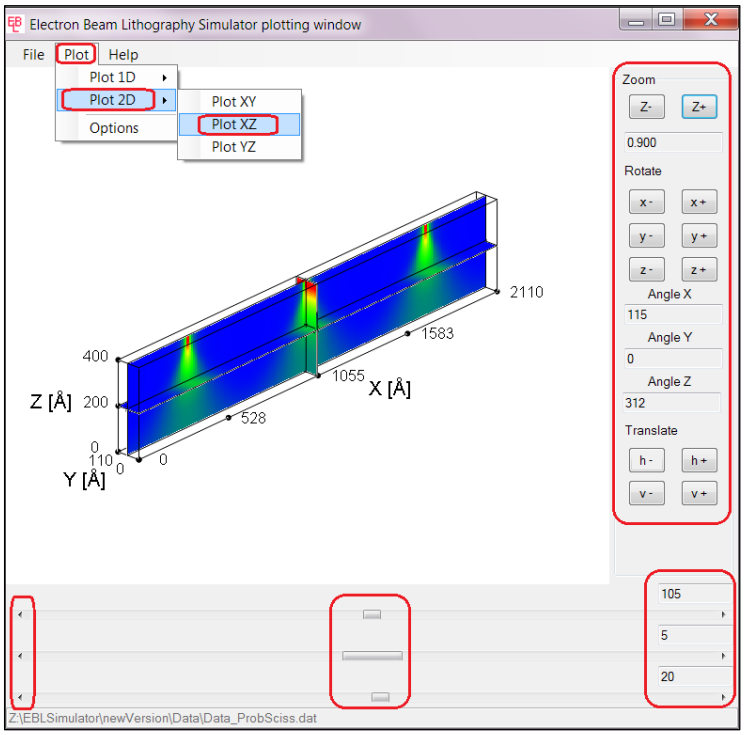

Figure 6: EBL Simulator Plotting window showing a computed 3D distribution of the scission yield in PMMA resist on Si substrate (the substrate is not shown).

1.7 The 2D Plot (XZ) of the scission yield is shown in Figure 7. The plot shows a cross-section of the scission yield distribution for the input grating geometry. The highest yield of scission occurs near the surface and decreases as the beam travels deeper into the resist. This trend is shown by color changing from red to blue.

Note 1.4: In 2D plots, the legend bar can be hidden by unchecking the box in **View/Legend Bar**, see Figure 8.

Note 1.5: In 2D plots, the scaling along vertical and horizontal axes can be synchronized by checking the box at **View/Proper aspect ratio**, see Figure 8.

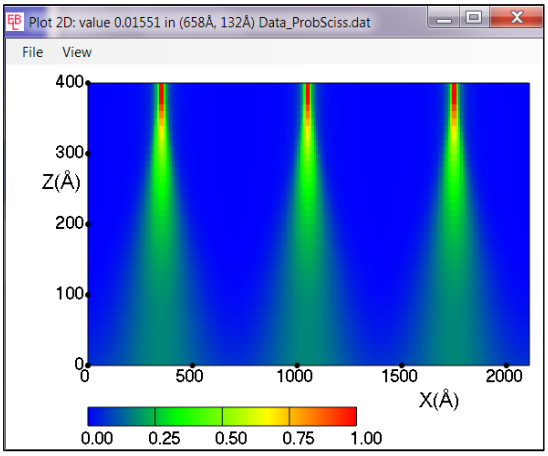

Figure 7: View of the cross section of 3D scission yield distribution in PMMA on a Si substrate, in a case of 1 keV exposure energy, 150 pC/cm line dose, 40 nm thick resist and 70 nm grating pitch.

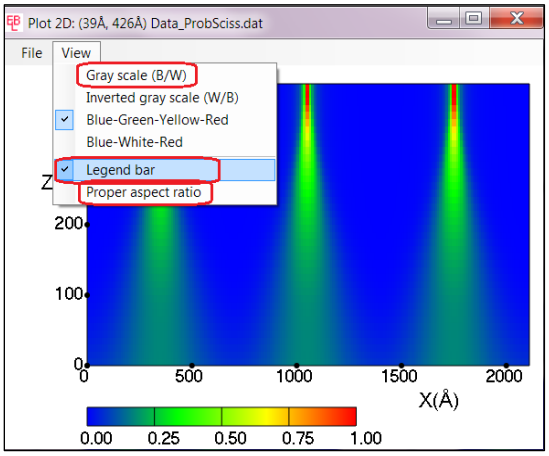

Figure 8: Selection of grayscale plot of the cross section of 3D scission yield distribution in PMMA on a Si substrate, in a case of 1 keV exposure energy, 150 pC/cm line dose, 40 nm thick resist and 70 nm grating pitch.

1.8 2D plots can also be visualized in color or in gray scale as shown in Figures 8 and 9. The plot window can be resized as required. The 2D Plot can be saved as a BMP, JPEG, or TARGA formats by selecting **File/Save as image** as shown in Figures 9 and 10.

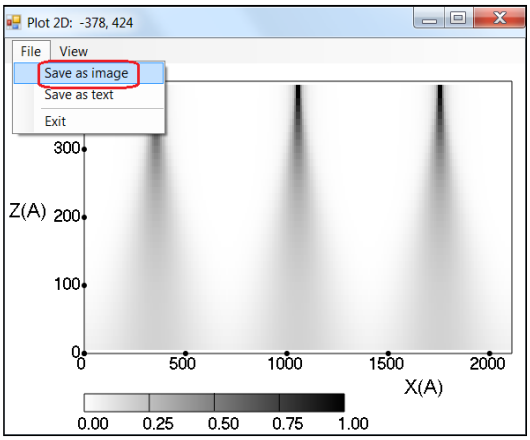

Figure 9: Gray scale view of the cross section of 3D scission yield from Figure 8.

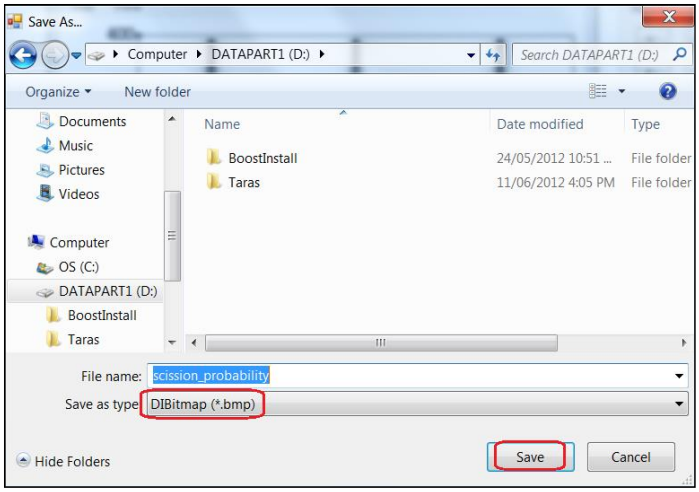

Figure 10: Save 2D Plot in Bitmap or TARGA format.

Note 1.6: Colors and legend bars in 2D plots represent relative levels of the yield of scission in fractions of the highest change of the function ($F_{max} - F_{min}$) that appears in the image. In 2D plots absolute values can be viewed in the title bar (see Figure 7) when moving the mouse.

Note 1.7: In order to output the absolute levels of the yield of scission, 1D plots should be used. The generation of 1D plots with examples can be found in the **Help** tool of the simulator, section **Plotting tool**.

2. Computation of Development Profiles

2.1 To compute development profile for an existing 3D distribution of the yield of scission in exposed resist, select **Development tab** as shown in Figure 11. You may select from **Resist** and **Developer** types. In this example, the default values for **PMMA** and **MIBK:IPA 1:3** are employed.

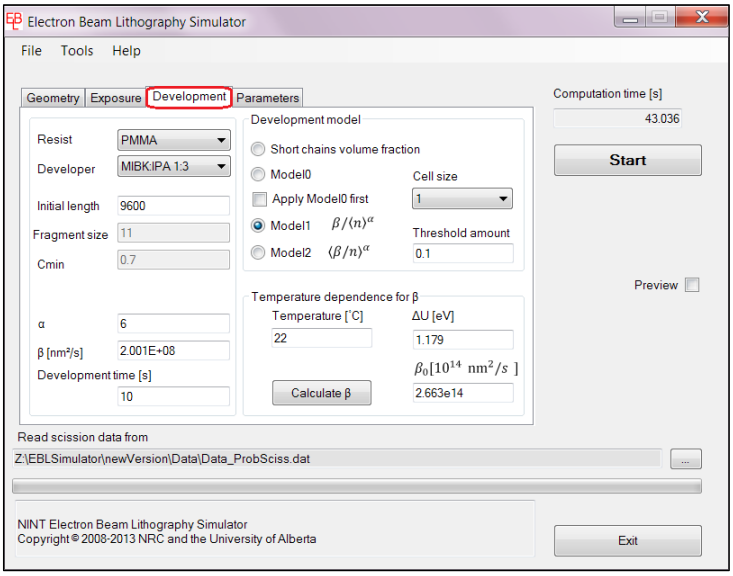

Figure 11: Main window of EBL Simulator: Development tab.

2.2 Select **Model 1** from the **Development model** block (Figure 12). To run the present example, enter –15°C for **Temperature.** Custom values of kinetic model parameters β_0 and ΔU may also be entered if so desired (see Note 3.3 below for the definitions). To run the present example, use the default values of parameters β_0 and ΔU that will appear in the boxes upon selecting **Model 1** as shown in Figure 12.

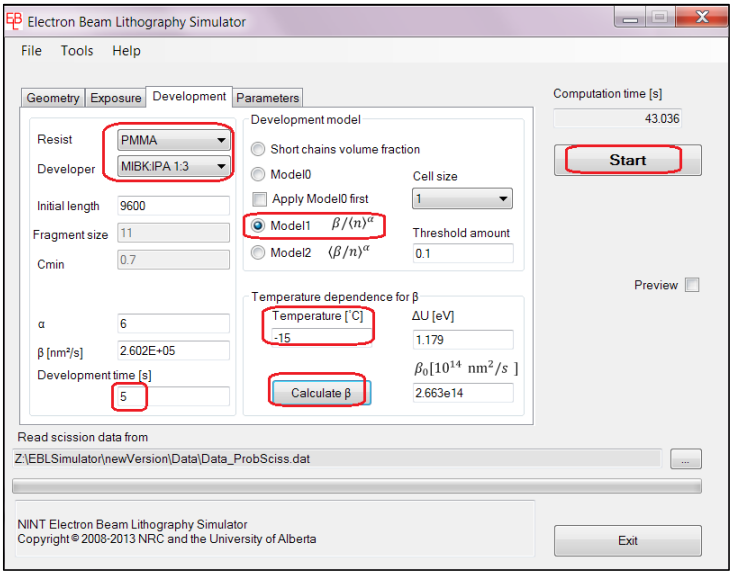

Figure 12: Settings for computing 3D development profile.

2.3 Click **Calculate β** button to compute the temperature dependent coefficient β to be used in the calculation (see Note 3.3 for the definition).

2.4 Enter **Development time** of 5 seconds.

2.5 You may change the file from which scission data will be read by clicking the button "**…**" in right bottom corner (Figure 12). By default, the file name corresponds to the last computed scission data file.

2.6 Click the **Start** button to run the computation. After clicking **Start**, **Save As** dialog window pops up. Enter a filename to save the 3D development profile and click **Save** button as shown in Figure 13.

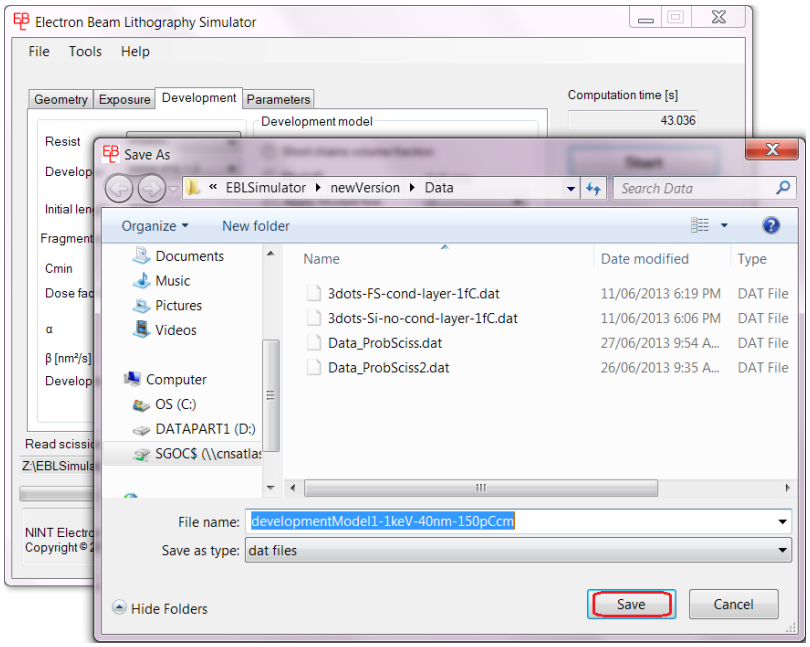

Figure 13: Specify a name for the 3D development profile data file.

2.7 To visualize the development profiles, select **Tools/Plot**. This opens the Plotting window. Select **File/Open** to load the development profile data for plotting as described in Sect. 1.3-1.7 and shown in Figures 4-6.

2.8 To View the 2D plots, Select **Plot** from the 3D Plot window **Plot 2D/Plot XZ** as shown in Figure 7

2.9 In 2D plots, spatial properties of the plot appear in the title bar when double clicking on the image or moving the mouse pointer while holding left mouse key.

Note 2.1: Time required to simulate development can be decreased by increasing **Cell size**. Since increasing the cell size makes the computations coarser, using **Cell size** of 1 nm is recommended for accurate predictions and 2nm or larger for quick approximate estimations.

Examples of Cold Development Profiles for 1 keV, 3keV and 10 keV Exposures at Various Times of Dissolution

2.10 Figure 14(a) shows a 2D Plot (XZ) of the clearance profile for an 1 kV exposure with PMMA thickness of 40 nm, line dose of 150 pC/cm and development for 1 second in an 1:3 MIBK:IPA mixture at -15˚C. To generate development profiles for 5 sec and 20 sec time of dissolution for the same conditions of exposure, repeat steps 2.1 - 2.7 replacing 1 sec development time with 5 sec and 20 sec, respectively. Development profiles for 5 sec and 20 sec dissolution time are shown in Figures 14(b) and 14(c), respectively.

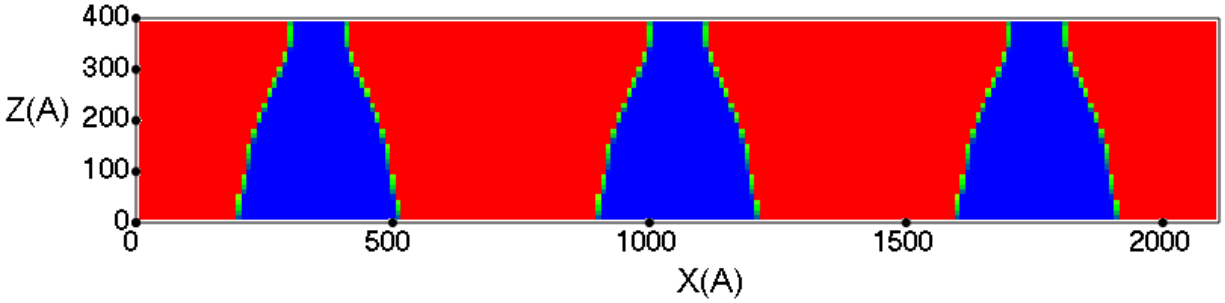

Figure 14(a): 2D plot of development profile of PMMA on a Si substrate, for the case of 1 keV exposure energy and 150 pC/cm line dose in a 40 nm thick resist, developed at -15˚C for 1 sec.

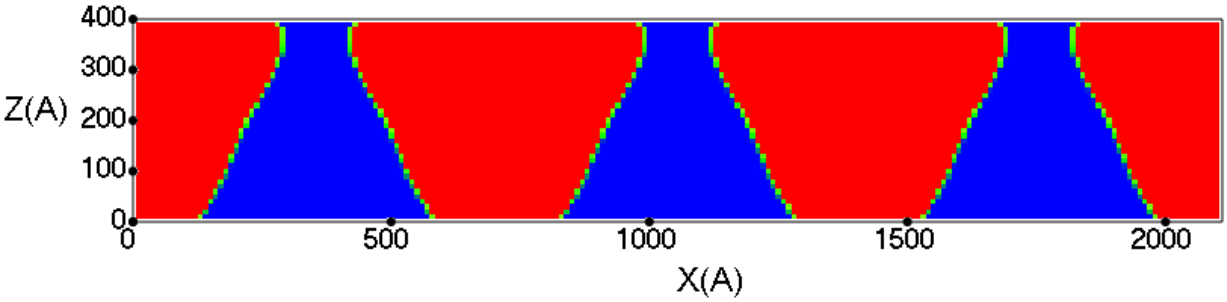

Figure 14(b): 2D plot of development profile for the case of 1 keV exposure energy and 150 pC/cm line dose in a 40 nm thick resist, developed at -15˚C for 5 sec.

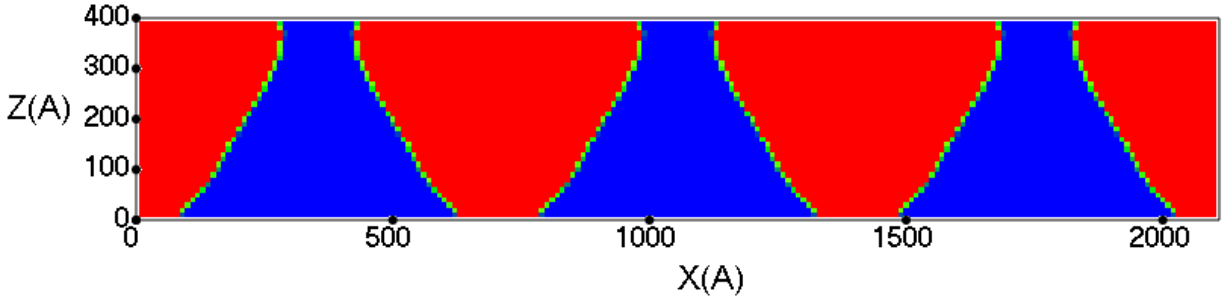

Figure 14(c): 2D plot of development profile for the case of 1 keV exposure energy and 150 pC/cm line dose in a 40 nm thick resist, developed at -15˚C for 20 sec.

Note 3.1: The colors in 2D plots represent the local volume fraction of remaining resist (PMMA) after development. Red indicates the remaining resist, and blue indicates the expected locations where the resist is cleared.

2.11 To simulate a 3 keV exposure of 55 nm thick resist with a line dose of 550 pC/cm, enter 3000 eV for exposure energy, 550 Å for resist thickness and 550 pC/cm for line dose and a pitch of 70 nm as shown in Figures 1 and 2. Following steps 1.1 - 1.7 will generate a 2D Plot (XZ) of the yield of scission as shown in Figure 15. To compute and visualize the development profiles for the computed yield of scission, repeat steps 2.1 - 2.7 using development times of 1 sec, 5 sec and 20 sec, respectively. The results are shown in Figures 16(a), 16(b), and 16(c) respectively.

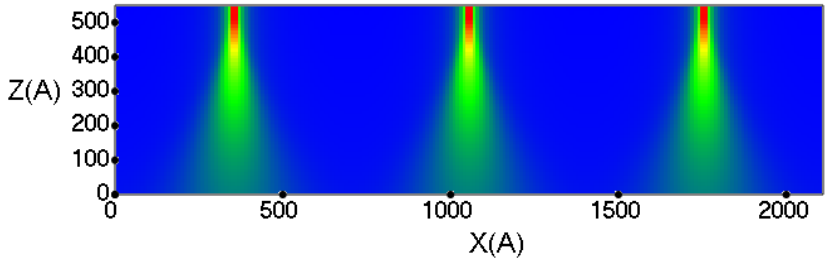

Figure 15: View of the cross section of 3D scission yield distribution in PMMA on a Si substrate, for a case of 3 keV exposure energy, 550 pC/cm line dose, and 55 nm thick resist, and 70 nm grating pitch.

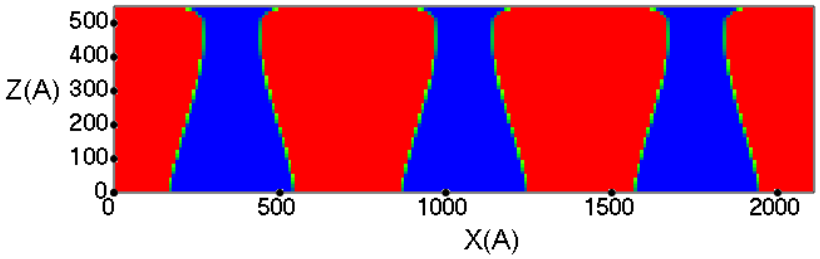

Figure 16(a): Development profile for the case of 3 keV exposure energy and 550 pC/cm line dose in a 55 nm thick resist, developed at -15°C for 1 sec.

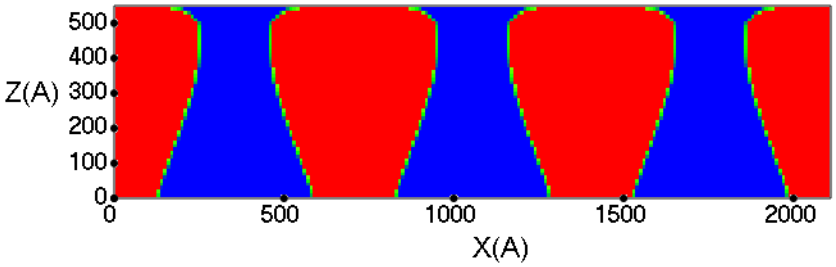

Figure 16(b): Development profile for the case of 3 keV exposure energy and 550 pC/cm line dose in a 55 nm thick resist, developed at -15°C for 5 sec.

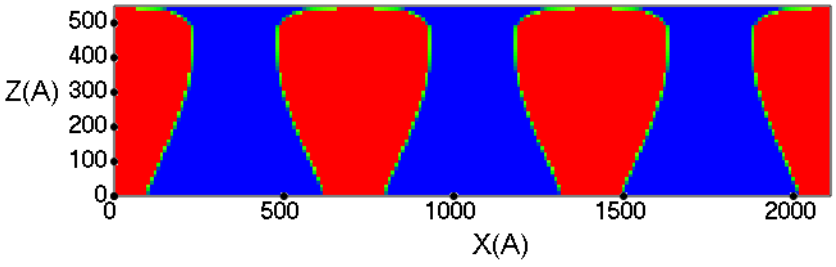

Figure 16(c): Development profile for the case of 3 keV exposure energy and 550 pC/cm line dose in a 55 nm thick resist, developed at -15°C for 20 sec.

2.12 To simulate a 10 keV exposure on a 55 nm thick layer with a line dose of 1500 pC/cm, enter 10000 eV for exposure energy, 550 Å for PMMA thickness, 1500 pC/cm for line dose, and a pitch of 70 nm as shown in Figure 1. Following steps 1.1 - 1.7 will generate a 2D Plot (XZ) of the yield of scission as shown in Figure 17. To compute and visualize the development profiles for the computed yield of scission, repeat steps 2.1-2.7 using development times of 1 sec, 5 sec and 20 sec respectively. The results are shown in Figures 18(a), 18(b), and 18(c) respectively.

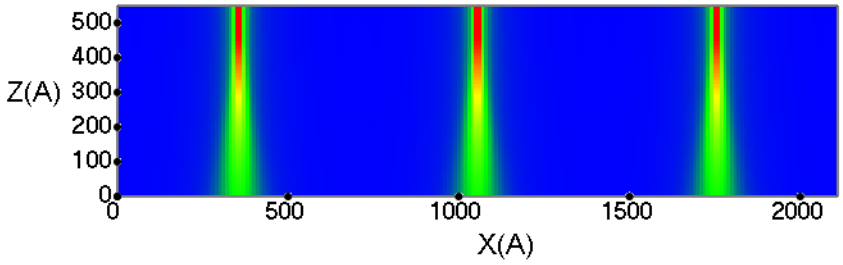

Figure 17: View of the cross section of 3D scission yield distribution in a case of 10 keV exposure energy, 1500 pC/cm line dose, 55 nm thick resist and 70 nm periodic gratings.

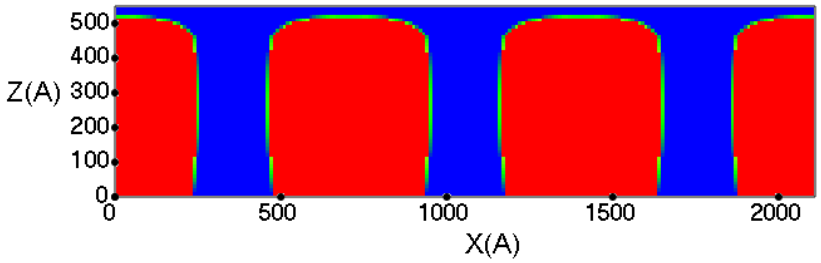

Figure 18(a): Development profile for the case of 10 keV exposure energy and 1500 pC/cm line dose in a 55 nm thick resist, developed at -15˚C for 1 sec.

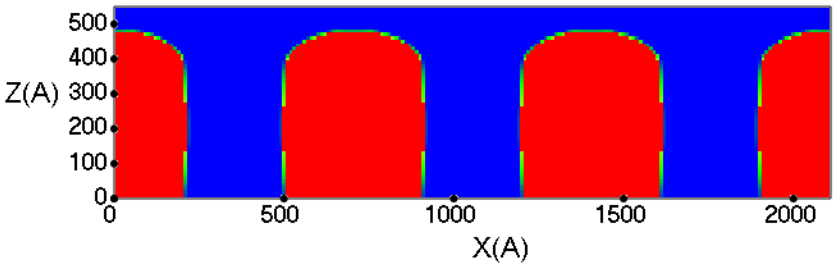

Figure 18(b): Development profile for the case of 10 keV exposure energy and 1500 pC/cm line dose in a 55 nm thick resist, developed at -15˚C for 5 sec.

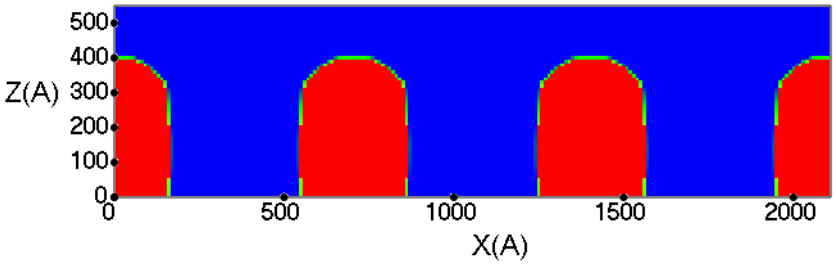

Figure 18(c): Development profile for the case of 10 keV exposure energy and 1500 pC/cm line dose in a 55 nm thick resist, developed at -15˚C for 20 sec.

Note 3.2:

In the simulator, the kinetic process of resist dissolution is represented by the motion of the resist-developer interface according to the equation[3,4,5,6]

$$\frac{dL}{dt} = D(x,y,z)L^{-1} \tag{1}$$

where $D(x,y,z)$ is the effective local diffusivity of fragments of exposed resist, and L is the depth of shrinking as a result of development. In this model, the rate of resist dissolution is a function of the entire history of the process of development, and thus depends on development time explicitly. This is different from the framework adopted in most if not all available models of EBL resist development, which assume the existence of a stationary regime that can be described by a constant rate of dissolution. In the simulator, the development model (1) is implemented as a sequence of discrete dissolution steps, where time δt required to dissolve a resist layer of thickness δL is determined by $\delta t = 2L\delta L / D(x,y,z)$ The simulation provides the location of the 3D resist-developer interface as a function of time of development. The clearance profiles seen in Figures 14, 16, and 18 represent the location of the resist-developer interface.

Note 3.3:

In development **Model 1** (used in the examples above), the effective local diffusivity of resist fragments $D(x,y,z)$ is determined by[6]:

$$D(x,y,z) = \frac{\beta}{\langle n \rangle^{\alpha}_{x,y,z}}, \tag{2}$$

where $\langle n \rangle$ is the average size of fragments of exposed resist at location (x,y,z), and the parameters α and β are constants and entered through the **Development** tab. The coefficient may be entered manually or computed accordingly to

$$\beta = \beta_0 \exp\left(-\frac{\Delta U}{kT}\right), \tag{3}$$

with β_0, ΔU, and T entered in the **Temperature dependence for β** block (see Figure 12).

In development **Model 2** the local diffusivity is given by[3,4,5]

$$D(x,y,z) = \left\langle \frac{\beta}{n^{\alpha(x,y,z)}} \right\rangle_{x,y,z}, \tag{4}$$

where n represents fragments of resist of different size and the averaging $\langle \rangle_{x,y,z}$ is performed over the local distribution of fragments that is derived from the 3D distribution of the yield of main chain scission. The power α is a function of the location and determined as follows,[3,4,5]

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[3] M.A.Mohammad, T. Fito, J. Chen, S. Buswell, M. Aktary, M. Stepanova, and S.K. Dew, Microelectronic Engineering, 87 (2010) 1104.

[4] M.A.Mohammad, T. Fito, J. Chen, S. Buswell, M. Aktary, S.K. Dew, and M. Stepanova, (2010). in: Lithography, Michael Wang (Ed.), ISBN: 978-953-307-064-3, INTECH, Available from: http://sciyo.com/articles/show/title/the-interdependence-of-exposure-and-development-conditions-when-optimizing-low-energy-ebl-for-nano-s?PHPSESSID=2s6gs1jtfkgkq5jio3hgpdups1.

[5] M. Stepanova, T. Fito, Zs. Szabó, K. Alti, A. P. Adeyenuwo, K. Koshelev, M. Aktary, and S. K. Dew, J.Vac. Sci. Technol. B. 28 (2010) C6C48 .

[6] M.A. Mohammad, K. Koshelev, T. Fito, D. Ai Zhi Zheng, M. Stepanova, and S. Dew, Jpn. J. Appl. Phys. 51 (2012) 06FC05.

$$\alpha(x,y,z)=\begin{cases}1+\langle n\rangle/n_0, & \langle n\rangle < n_0\\ 2, & \langle n\rangle \geq n_0\end{cases}, \qquad (5)$$

where n_0 is entered through the **Development** tab (upon selecting **Model 2** $\boldsymbol{\alpha}$ text box turns into $\boldsymbol{n_0}$ text box).

Note 3.4:
Parameters α, n_0, β_0, and ΔU can be evaluated by fitting the computed percentages of resist left on the substrate to the corresponding experimental results[5,6]. The default values for α, β_0, and ΔU in **Model 1** (Figure 12) have been obtained from experimental contrast curves of PMMA developed in a 1:3 MIBK:IPA and 3:7 IPA:Water mixtures, and for ZEP520A developed in ZEDN50 and 1:3 MIBK:IPA mixtures. It should be noted however, that these parameters are not precisely determined and their variation may be acceptable. Users can custom-tune the dissolution parameters if so desired. See also Note 4.1 in Part IV on tuning of the development parameters.

Note 3.5:
Solvents other than the supported ones can be employed to develop PMMA or ZEP resists, given that the corresponding development parameters are available. To use a custom developer, select a developer in the **Developer** drop-down menu and enter the applicable development parameters.

Note 3.6:
The levels of diffusivity may be output by using **Tools/Diffusivity analyzer** menu item. The tool allows computing the effective average diffusivity of resist fragments at location (x,y,z), using as the input existing 3D distributions of the scission yield in exposed resist, see **Help** tool for further instructions.

Note 3.7:
Negative tone resists are not supported by the models of development included in the present version of the simulator.

II. Thick Resist Layers and Increased Exposure Voltages

Below examples are described for computation of exposure, fragmentation, and development in 300 and 600 nm thick layers of **PMMA**, on a Si substrate using 10 keV and 30 keV beam voltages, see also Table 1. The examples are given for periodic gratings with a 200 nm pitch.

Table 1. Settings for EBL exposure simulation in this example.

E0 [keV]	Line dose [pC/cm]	Line spacing [Å]	Thickness [Å]	CW [Å]	BSSS [Å]
10	1000, 1500	1980	3000	3000	200
30	1000, 2000	1980	3000	1000	200
30	4000	1980	6000	4000	200

1. Simulation of Exposure

1.1. Launch the simulator.

1.2. In the **Geometry** tab check the **Periodic** box (all cases in this section are calculated with periodic conditions applied) and set **Line spacing** to 1980 Å. The writing geometry may be visualized by clicking on the **Plot geometry** button. An example of geometry for a periodic grating is shown in Figure 19(a).

1.3. Switch to **Exposure** tab and set appropriate conditions, **Exposure energy** (electron beam voltage), exposure **Line dose**, and **Resist thickness** (see Table 1 and Figure 19b). The remaining parameters of this tab are taken by default.

1.4. In **Parameters** tab, set **Computational window V/H** and **Backscattering step size** parameters according to Table 1 (CW and BSSS, respectively, see also Figure 19c). The other parameters in this tab are taken by default.

1.5. To run the simulation, click on **Start** button. This will turn its label from **Start** into **Stop exposure**. After the computation is completed, the 3D spatial distribution of the yield (probability) of main chain scission will be saved. The reset of **Stop exposure** label is the indication that the computation is completed.

Note 1.1: If so desired user can increase **Backscattering step size** beyond 200 Å to decrease time of computations at high exposure energies in 50-100 keV voltage regimes (not required in this example).

Note 1.2: If **Computational window** is insufficient for the resist thickness selected, warning message "Computational window size is too small" will appear containing also a recommended value of **Computational window V/H** to be entered through **Parameters** tab.

Note 1.3: User may choose the filename for the 3D distribution of scission yield (probability) by clicking the "**...**" button in the main window. By default the file is written in the **Data** folder created automatically in the folder from where the simulator is run, in the file **Data_ProbSciss.dat**. To avoid overwriting existing files, it is recommended to change name of the output file before running a new calculation.

Note 1.4: Clicking the **Plot geometry** button activates a **Geometry viewer** pop-up window that shows the current writing geometry (Figure 19a). Horizontal (H) and vertical (V) parameter settings correspond to the respective directions in the **Geometry viewer** window.

Note 1.5: The 3D yield of scission and also 2D cross-sectional profiles can be visualized and saved using the **Tools/Plot** instrument as described in **Part I** of this manual and in the **Help** tool. The 2D cross section views of scission yield for the sets of parameters from Table 1 are shown in Figures 20(a, b, c).

Note 1.6: The legend bar in Figures 20(a, b, c) indicates the relative levels of the yield of scission in fractions of the highest value ($F_{max} - F_{min}$) appearing in the image. To output the absolute levels of the yield, 1D plots should be used as described in the **Help** tool of the simulator.

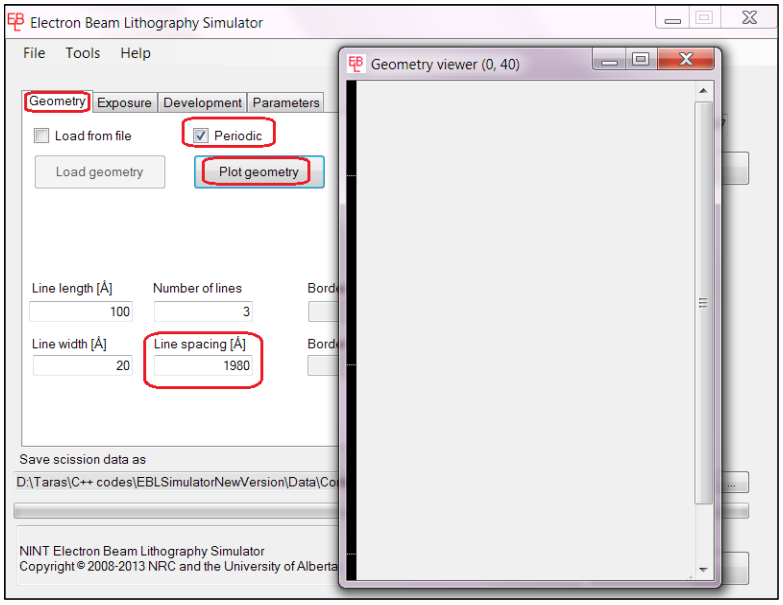


Figure 19(a). Geometry tab of EBL Simulator with Geometry viewer window open.

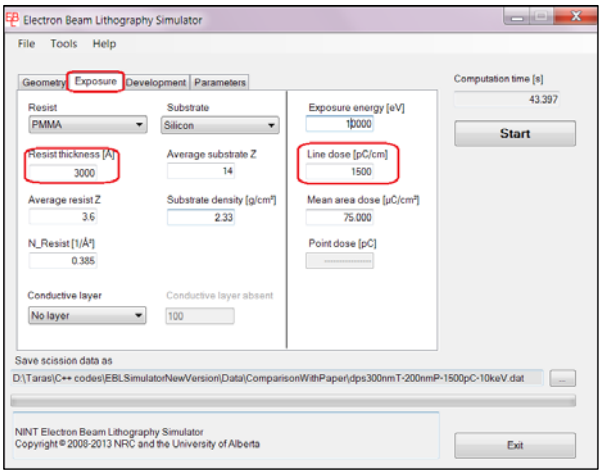


Figure 19(b). Exposure tab.

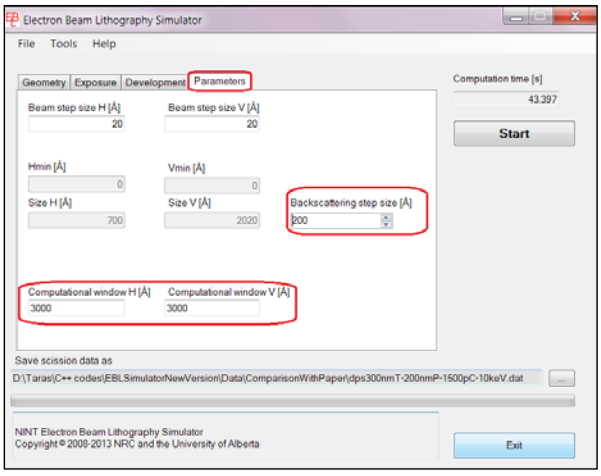


Figure 19(c). Parameters tab.

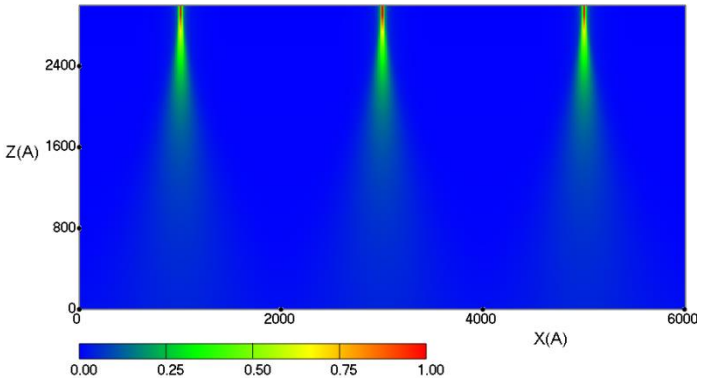


Figure 20(a). 2D plot of the 3D scission yield distribution in a periodic grating for the case of 10 keV exposure energy and 1500 pC/cm dose in a 300 nm thick PMMA on a Si substrate (not shown).

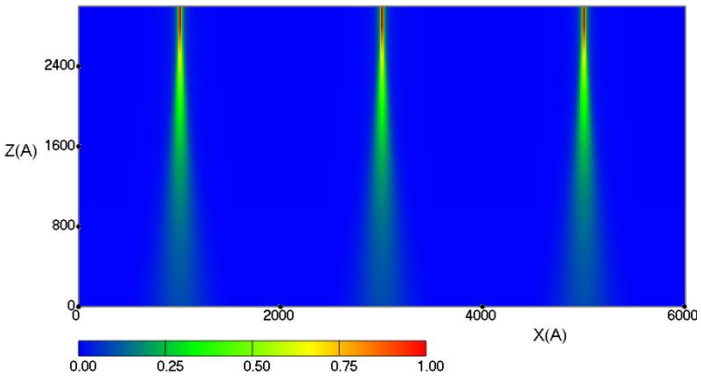


Figure 20(b). 2D plot of the 3D scission yield distribution in a periodic grating for the case of 30 keV exposure energy and 4000 pC/cm dose in a 300 nm thick resist on a Si substrate.

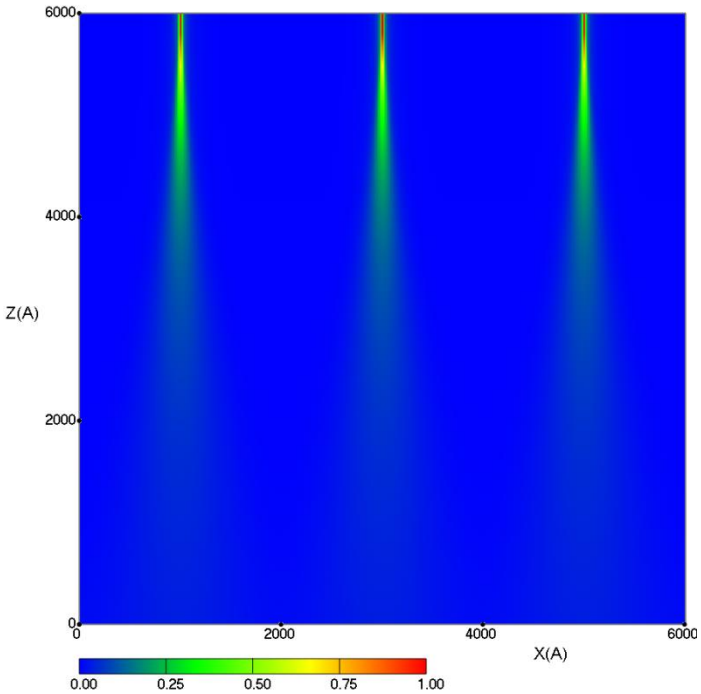


Figure 20(c). 2D plot of the 3D scission yield distribution in a periodic grating for the case of 30 keV exposure energy and 4000 pC/cm dose in a 600 nm thick resist on a Si substrate.

2. Working with Exposure Dose Convertor

Simulation of the yield (probability) of scission may be a computationally intense task. Several different factors contribute to the increase of the time of computation, such as high exposure voltage, high thickness of the resist, as well as size and shape of the writing pattern. However, in certain cases it is possible to reduce the computation time. In particular, when it is desired to generate a set of results with different exposure doses whereas other parameters are unchanged, it is sufficient to run the simulator only once in order to generate a 3D distribution of the yield of scission for one reference exposure dose. The distributions corresponding to other doses may be obtained using the **Dose convertor** tool. The steps are as follows:

2.1. Select **Tools/Dose convertor**.
2.2. Specify appropriate 3D scission yield distribution file in **In file** edit window by applying "**…"** button. By default, the last generated file is used for output. In **Out path** edit window, specify filename of the output file.
2.3. Enter the factor of conversion in the **Factor:** edit box. For example, if it is desired to increase the exposure dose by 2.5 times, the number 2.5 should be entered.
2.4. Click on the **Convert** button. The label will change into **Wait please.** The reset of the **Convert** label indicates the end of the conversion.

Note 2.1: The dose conversion can be applied to scission yield distributions only. The conversion is not applicable to other outputs of the simulator, which are nonlinear functions of exposure dose.

3. Computation of Development Profiles

After a desired set of scission yield (probability) files is generated, the next step is to simulate the process of development and compute the clearance profiles in the resist by applying an appropriate model of dissolution. This may be done as follows:

3.1. Open the main window.
3.2. Switch to **Development** tab (Figure 21).
3.3. Chose the appropriate model of dissolution and set parameters for the model. In the examples below, **Model 1** is used (Figure 21).
3.4. Click on **Start** button. After this the button's label turns into **Stop development** and the progress bar appears showing the progress. The reset of **Start** indicates that the calculation is over.

Note 3.1: Calculation may be aborted by pressing the **Stop development** button while calculation runs.

Note 3.2: Both the yields of scission and development profiles are calculated in the background regimes, i.e. during that time user is able to do other jobs with the simulator, for example plot images of previously computed structures, etc.

Note 3.3: Examples of development profiles for periodic gratings (shown in the form of 2D cross sections of the corresponding 3D distributions) are presented in Figure 22(a, b) and Figure 23(a, b). The profiles in Figures 22 and 23 are different only in the exposure doses applied.

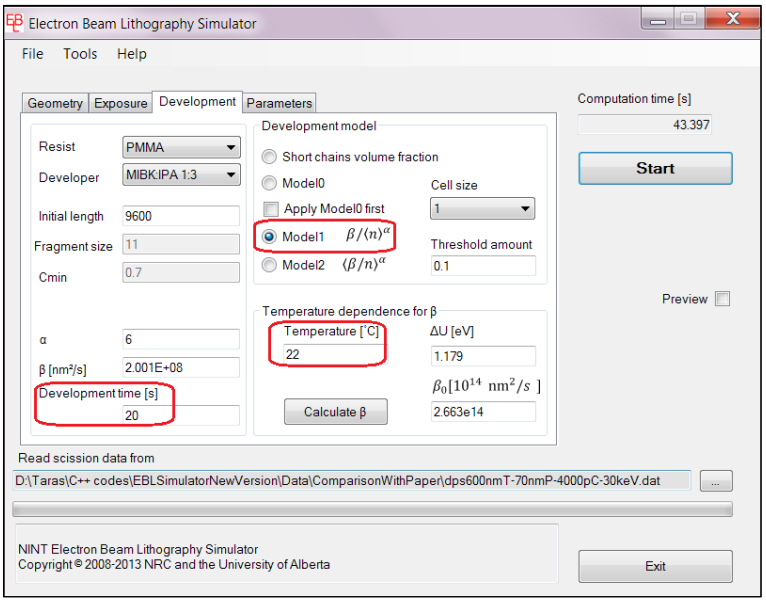


Figure 21. Development tab of EBL Simulator.

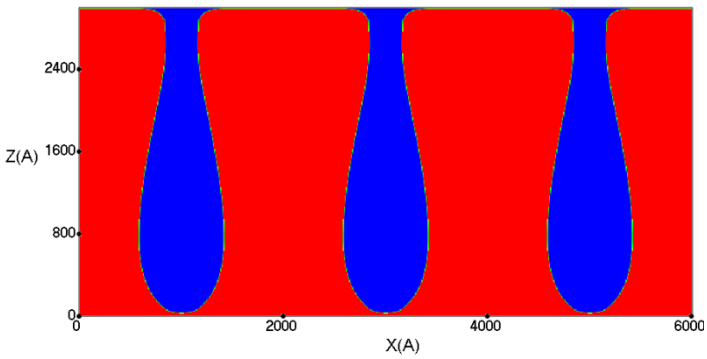


Figure 22(a). 2D plot of the development profile for the case of 10 keV exposure energy and 1000 pC/cm dose in a 300 nm thick PMMA resist, developed in a 1:3 MIBK:IPA mixture during 20 s at temperature 22˚C.

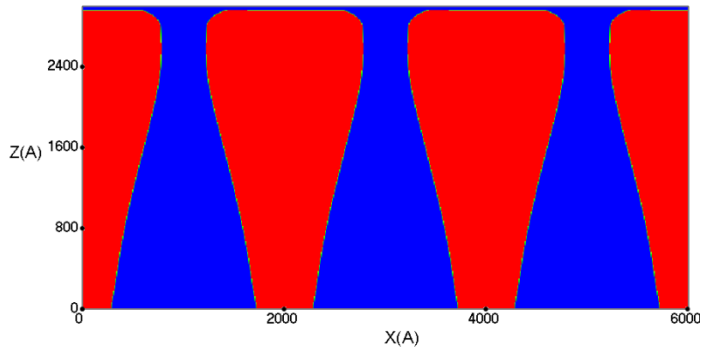


Figure 22(b). 2D plot of the development profile for the case of 10 keV exposure energy and 1500 pC/cm dose in a 300 nm thick PMMA resist, developed in a 1:3 MIBK:IPA mixture during 20 s at temperature 22˚C.

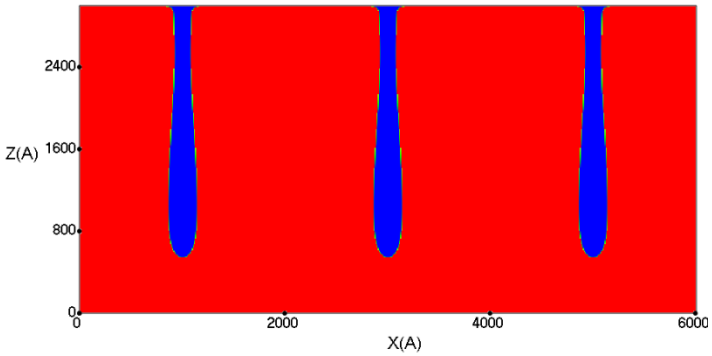


Figure 23(a). Development profile for the case of 30 keV exposure energy and 1000 pC/cm dose in a 300 nm thick PMMA resist, developed in a 1:3 MIBK:IPA mixture during 20 s at temperature 22˚C.

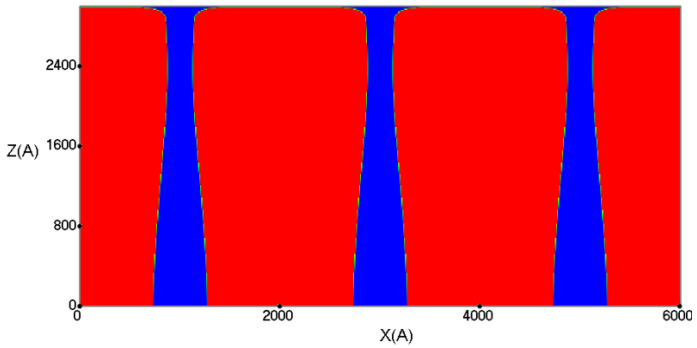


Figure 23(b). Development profile for the case of 30 keV exposure energy and 2000 pC/cm dose in a 300 nm thick PMMA resist, developed in a 1:3 MIBK:IPA mixture during 20 s at temperature 22˚C.

4. Changing the Temperature of Development

One of purposes of the simulator is to facilitate the understanding of the trends that determine the process of development at the nanoscale. A parameter which has a major influence on the dissolution process is temperature of development. In order to vary the temperature of development, execute the following steps:

4.1. Open the main window of the simulator.
4.2. Select the **Development** tab and choose **Model 1** or **Model 2**.
4.3. Enter the appropriate temperature in the **Temperature** edit box and click on the **Calculate β** button. Calculated parameter **β** will appear in the corresponding edit box.

5. Changing the Development Time

One more parameter of major importance is the time of resist development (dissolution). In order to change the dissolution time:

1. Open the main window of the simulator.
2. Switch to the **Development** tab and select **Model 1** or **Model 2**.
3. Set the dissolution time in the **Development time** edit box.
4. Click on the **Start** button.

6. Examples of Development Profiles in a Thick Layer of PMMA

Examples of development profiles for periodic grating with a 200 nm pitch in a 600 nm thick resist (cross sections of the corresponding 3D distributions) shown in Figures 24 and 25 differ in temperature of development with other conditions unchanged, whereas Figures 26 and 28 differ in time of dissolution with other conditions unchanged. Using such simulations, the dependence of the clearance profile on the major EBL process parameters may be investigated.

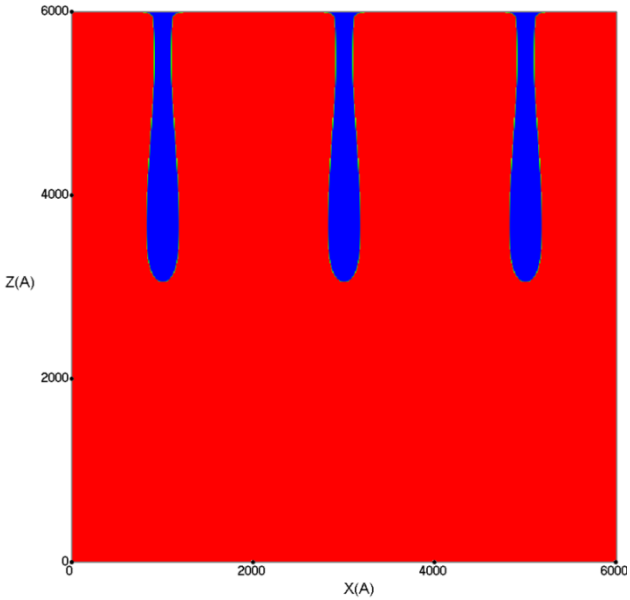


Figure 24. Development profile for the case of 30 keV exposure energy and 4000 pC/cm dose in a 600 nm thick PMMA resist, developed in a 1:3 MIBK:IPA mixture during 20 s at temperature -15˚C.

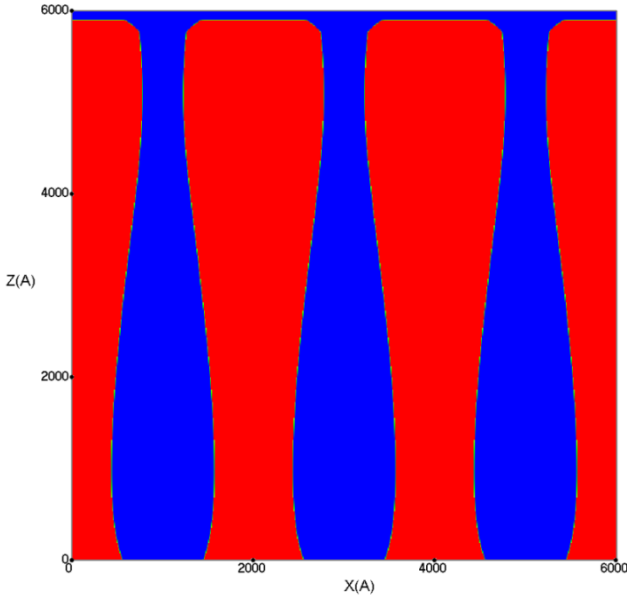


Figure 25. Development profile for the case of 30 keV exposure energy and 4000 pC/cm dose in a 600 nm thick PMMA resist, developed in a 1:3 MIBK:IPA mixture during 20 s at temperature 22˚C.

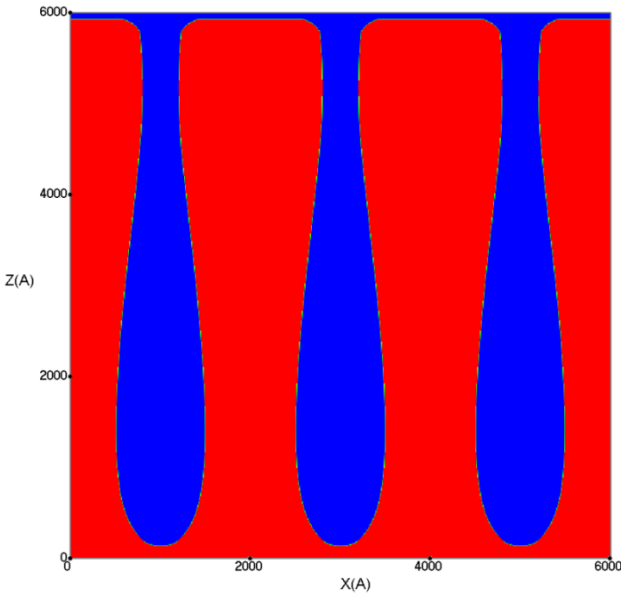


Figure 26. Development profile for the case of 30 keV exposure energy and 4000 pC/cm dose in a 600 nm thick PMMA resist, developed in a 1:3 MIBK:IPA mixture during 10 s at temperature 22˚C.

III. Usage of Graphical Geometry Input: Example for Modeling the Resonator Clamping Point

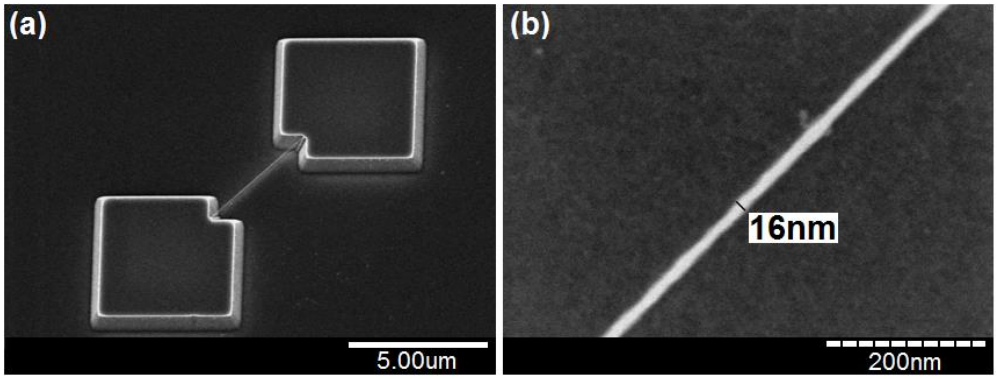


Figure 27. A suspended 16nm wide and 5um long SiCN resonator on Si bases, (a) overview image, and (b) magnified image of the bridge[1].

Here we describe a simulation of the EBL process that we have employed to fabricate the suspended silicon carbon nitride (SiCN) **bridge resonator structures** on a silicon substrate as shown in Figure 27.[1] In order to fabricate such structures, the initial mask was a 45 nm thick single layer of PMMA. **Low-voltage exposure** (3 keV) was employed with the geometry design as outlined in Figure 28 and Table 2. **Cold development conditions** (–15°C) were used.

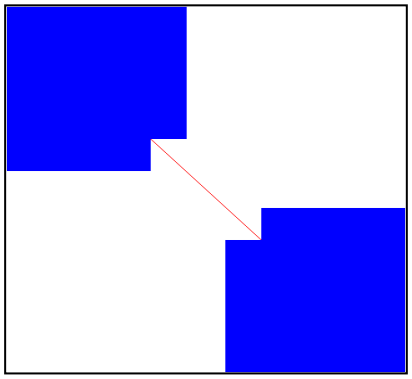


Figure 28. Sketch of the EBL exposure design used to fabricate the resonator structure.

Table 2. Selected dimensions and process parameters

Structure	Exposed as	Clearance Dose
Pads (5µm x 5µm)	Areas	600 µC/cm^2
Bridges (20nm x 2.5µm)	Single Pixel Lines	1125 pC/cm

[1] M.A. Mohammad, C. Guthy, S. Evoy, S.K. Dew, and M. Stepanova, *J. Vac. Sci. Technol. B* **28**, C6P36 (2010).

1. Creation of Input Graphic File Representing the Clamping Area

1.1. Of major interest is simulation of the *clamping area* of the resonator structure, i.e. the area where the nanoscale bridge structure meets the large exposed pad. To simulate the clamping area, a suitable graphic file (BMP, TIF, or JPG) must be created that would identify the writing geometry and doses applied. An example input image is shown in Figure 29.

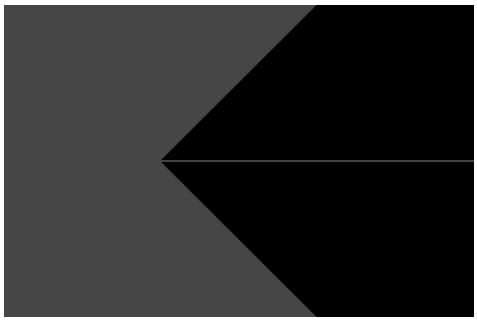


Figure 29. The input image showing the clamping point of the bridge structure[1].

1.2. Generally, the design shown in Figure 29 would require the application of both area and line doses (see also Table 2). However, images used as input to the EBL simulator employ point doses only. Every pixel in the image correspond to 1 nm^2, and the levels of grey correspond to the *relative* dose applied to every point, according to the following rule:

- Black – RGB 0, 0, 0 – No dose applied.
- White – RGB 255, 255, 255 – Maximum dose applied.

The user can differentiate the relative local dose levels by using 256 levels of grey. Thus if one requires a level of 25% relative to the maximum dose for a particular structure, then the corresponding local RGB should be set to 64, 64, 64. The maximum point dose employed in the structure is set in the main window of the simulator as described in sect. 2.1.

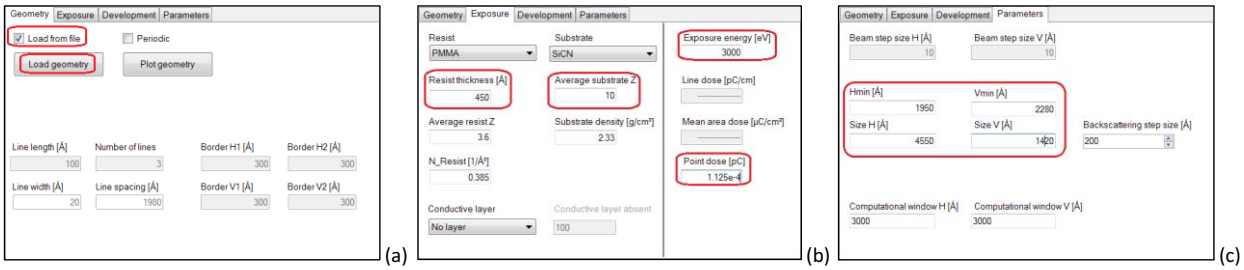
1.3 In Figure 29, the levels of grey may be obtained from the data given in Table 2 as follows:

Point dose for bridge (PDB):
1125 pC/cm = 1.125×10^{-4} pC/nm; since 1 pixel = 1nm × 1nm → 1.125×10^{-4} pC/nm^2
Point dose for pad (PDP):
600 $\mu C/cm^2 \times (10^{-7})^2$ $cm^2/nm^2 = 6.0 \times 10^{-18}$ $C/nm^2 = 6.0 \times 10^{-6}$ pC/nm^2
Point dose for pad relative to point dose for bridge (PDP/PDB):
$6.0 \times 10^{-6} / 1.125 \times 10^{-4} = 0.05333$
Level of grey for bridge:
RGB 255,255,255. This corresponds to the maximum point dose employed in the structure.
Level of grey for pad:
RGB 14, 14, 14. This corresponds to 0.05333 times the maximum point dose applied.

Note 1.1: The level of grey RGB 14, 14, 14 that must be applied to the pad in the calculations produces a very dark grey shade. In order to make the pad in Figure 29 visible, the pad was false-coloured by using a lighter shadow of grey. This change of grey shade is done solely for the visualization purposes and does not affect the simulations described below.

2. Working with the Graphical Input

2.1. Open the main window of the simulator. To import the graphic file, check the **Load from file** check box as shown in Figure 30(a). This will enable the **Load geometry** button, clicking on which will pop-up a dialog window for specifying the path to the graphic input file. Once the graphic input file is uploaded, clicking on the **Plot geometry** button creates a **Geometry viewer** pop-up window visualising the graphic input file as shown in Figure 31(a).

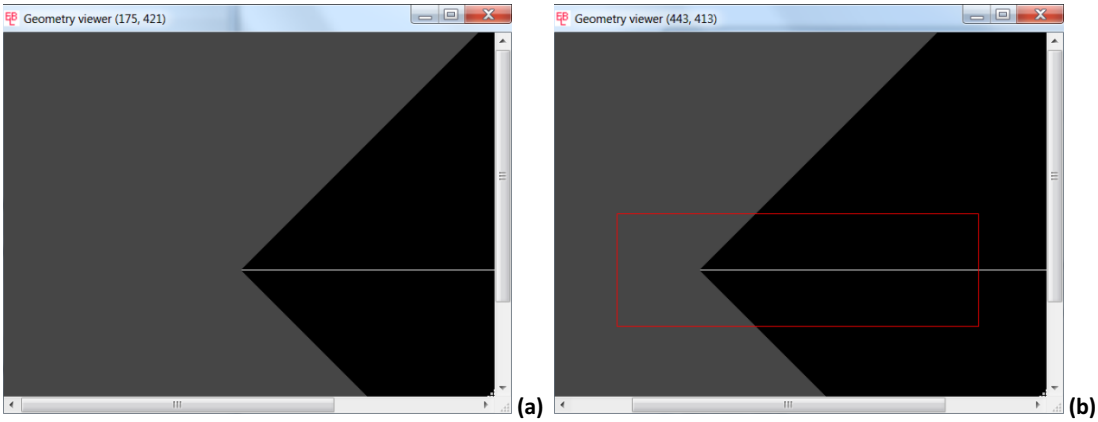


(a) (b) (c)

Figure 30. Usage of Geometry tab (a), Exposure tab (b) and Parameters tab (c) of EBL Simulator.

2.2. The simulator allows performing computations in a selected part of the uploaded pattern. The computational box can be set up in two ways: (i) with mouse, by right clicking and selecting the desired area in the window **Geometry viewer**, or (ii) by entering the boundaries in the **Hmin**, **Vmin**, **Size H** and **Size V** edit boxes in the **Parameters** tab, see Figure 30(c). In case (ii), the **Plot geometry** button must be pressed again to visualize the computational box, which will be indicated by thin red lines as shown in Figure 31(b).

Note 2.1: Usage of a smaller computational box is highly recommended since this decreases the time of computations. All proximity effects due to electrons from the surrounding areas are accounted for when the simulation is run within a smaller box such as shown in Figure 31(b). For consistent results the boundaries of the original graphic image must be a certain distance away from the computational box. This distance depends on the extent of the proximity effect, which depends on the voltage, and may vary from a few hundred nanometres to micron-scale distances.



(a) (b)

Figure 31. Plot of the graphic file (a), and the computational box around the clamping point (b).

3. Simulation of Exposure and 3D Visualization of Computed Profiles.

3.1. After the graphic image is uploaded and the computational box selected, user must enter **average substrate Z** and **substrate density**, **Resist thickness**, and conditions of exposure (**Exposure energy** and the maximum **Point dose**) through **Exposure** tab of the simulator (see Figure 30(b)). In drop-down **Substrate** list select **Customize** and enter **Substrate name**, **Average substrate Z,** and **Substrate density**. In the present example, **average substrate Z** equal to 10 and **substrate density** equal to 2.33 g/cm^3 are used. After clicking the **Start** button, the yield of scission will be computed and saved. The **Plotting Window** can be used then to view the yield of scission profile as shown in Figure 32. By using the zoom, tilt, and translate buttons on the side and the XYZ plane buttons on the bottom, as well as by changing the number of XYZ ticks through the **Plot**/**Options** drop down menu item, a desired appearance of the image can be reached. Moving the sliders at the bottom of the window would select the desired cross-sections for visualization.

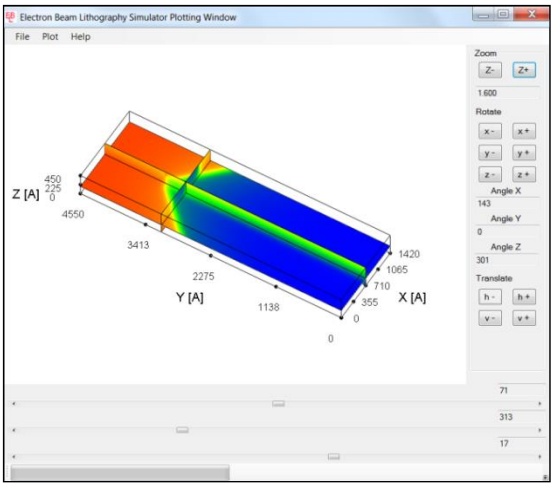


Figure 32. EBL Simulator plotting window showing the 3D profile of the yield of scission in the resist.

3.2. 3D images may be saved using the **File/Save Figure** drop down menu item in the plotting window. This will invoke a pop-up dialog window prompting the user to save the file at a desired location in BMP, JPG, or TGA formats. Figure 33(a) shows an example of saved 3D image.

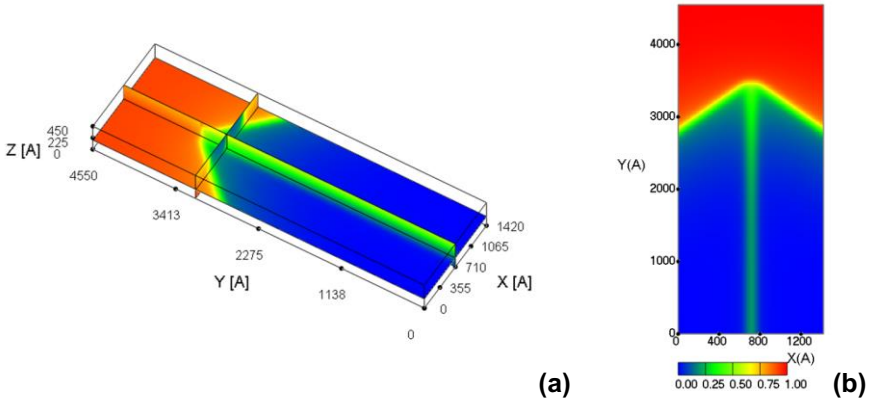


Figure 33. (a) – 3D visualization of the probability of scission;
(b) – 2D (XY) cross-sectional plot of the yield of scission from (a).

3.3. To generate a two dimensional (2D) cross-sectional plot of the 3D data, the **Plot/Plot 2D** drop down menu item should be used in the plotting window. The position of the cross-sections may be selected by using the sliders in the bottom of the plotting window. The image may require a size adjustment by manually dragging the window boundaries in order to reach appropriate visual aspect ratio. An example of a 2D (XY) cross-sectional plot of the probability of scission is shown in Figure 33(b). The legend bar in the Figure represents the relative levels of the probability of scission in the 2D image.

4. Computation of Development Profile using Cold Development Conditions.

4.1. After the 3D distribution of the yield (probability) of scission is computed and saved, the corresponding development profile can be generated using the **Development** tab. Once the appropriate probability of scission file has been loaded, the correct model and parameters need to be selected. This case study involves development at a decreased temperature (–15°C), for which user should select **Model1** as shown in Figure 34 below. This model enables edit boxes in the **Temperature dependence for β** block. By entering the desired development temperature and clicking on the **Calculate β** button, the value of model parameter **β** corresponding to the selected temperature is instantly loaded into the corresponding box. After clicking **Start** and indicating the output path, the 3D development profile is generated as shown in Figure 35.

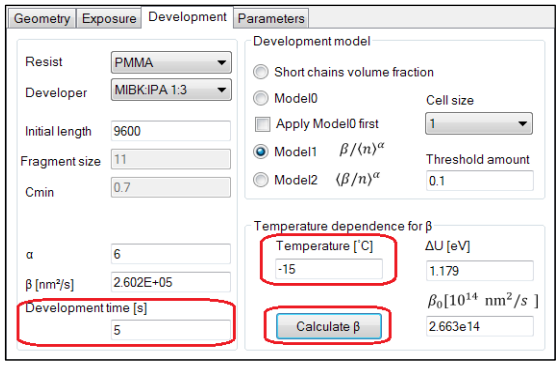


Figure 34. Model and parameter selection for computation in Development tab.

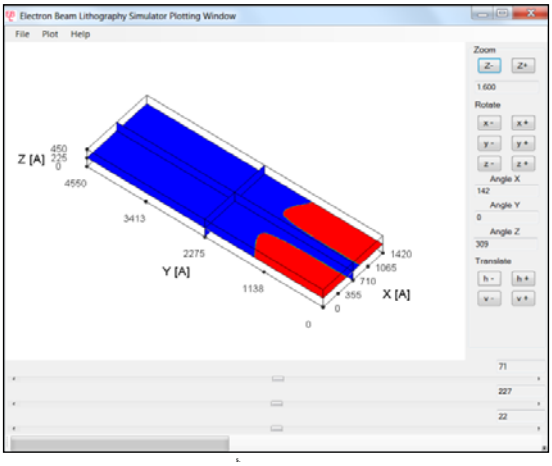


Figure 35. EBL Simulator plotting window showing the computed 3D development profile of the resist.

5.1. To generate the corresponding 2D XY and XZ plots of the 3D profile, the **Plot/Plot 2D/Plot XY** and **Plot/Plot 2D/Plot XZ** drop down menu items should be used in the plotting window. This will generate images as shown in Figure 36(a) and (b) respectively (after setting appropriate image dimensions with mouse manipulator).

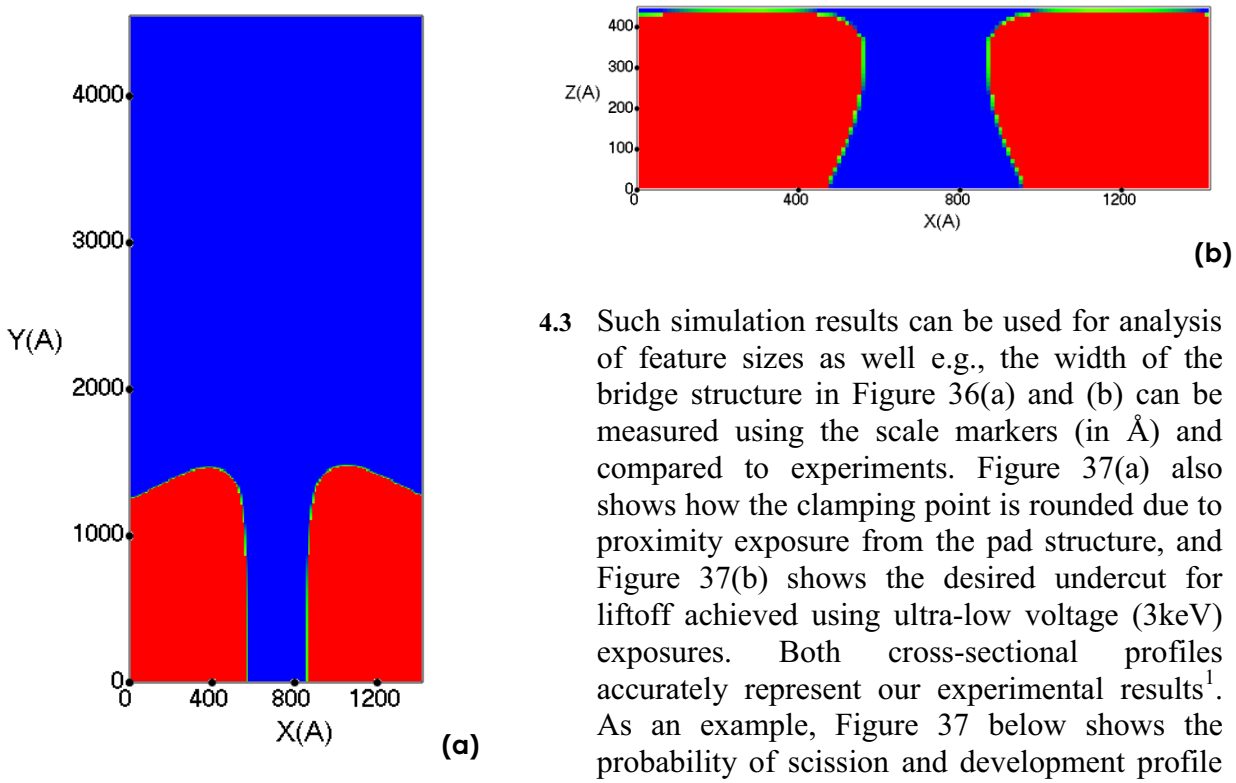


Figure 36. XY (a) and XZ (b) cross-sections of 3D development profile from Figure 35.

4.3 Such simulation results can be used for analysis of feature sizes as well e.g., the width of the bridge structure in Figure 36(a) and (b) can be measured using the scale markers (in Å) and compared to experiments. Figure 37(a) also shows how the clamping point is rounded due to proximity exposure from the pad structure, and Figure 37(b) shows the desired undercut for liftoff achieved using ultra-low voltage (3keV) exposures. Both cross-sectional profiles accurately represent our experimental results[1]. As an example, Figure 37 below shows the probability of scission and development profile images of the clamping point compared with the SEM image of the fabricated device.

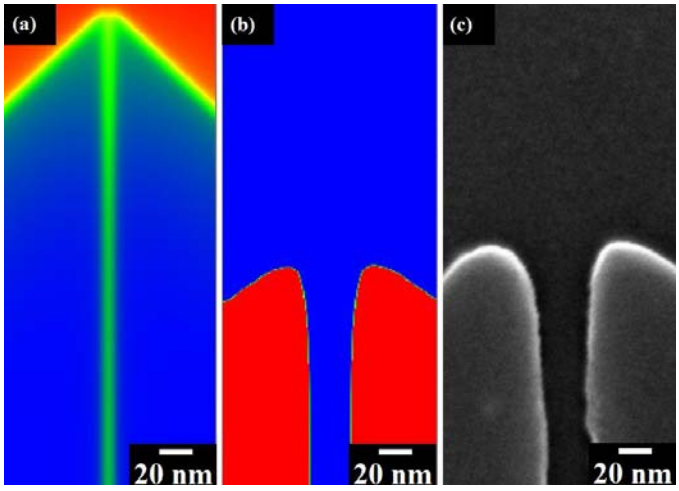


Figure 37. Computed probability of scission (a), and development profile (b), compared with experimental SEM image (c) of the developed clamping point area[1].

IV. Contrast Curves

Contrast curves are employed broadly to characterize the sensitivity and contrast of EBL process. To obtain contrast curves, a large area of resist is exposed uniformly with various doses, and the resist's thickness after development is plot as a function of the exposure dose. Here examples are given of contrast curve calculations for PMMA and ZEP resists at the conditions that match the experiments [1,2] employed for comparison.

1. Exposure settings for PMMA resist on Si substrate

1.1. Prepare graphical file (BMP, TIF, or JPG) with size 80×80 pixels, which corresponds to a 80 nm × 80 nm area. Fill the entire area with white color.

1.2. Launch the simulator. In the **Geometry** tab, check **Load from file**, load the graphical file, and check the **Periodic** checkbox to simulate a large exposure area.

1.3. In the **Exposure** tab, select **PMMA** in the corresponding drop-down menu list and enter the value of **Resist thickness** equal to 2770 Å. Next, enter **Point dose** equal to 10^{-6} pC/pixel. For this, type "1E–06" in the corresponding edit box. Since a pixel represents one square nanometer, the point dose of 10^{-6} pC/pixel corresponds to the area dose of 100 μC/cm^2. Make it sure that correct substrate atomic number and density (14 and 2.33 g/cm^3, respectively, for Silicon) appear in the corresponding edit boxes.

1.4. Since the resist layer is relatively thick, the computational window in the **Parameters** tab needs to be increased (see **Help** for the definition of this parameter). In the **Parameters** tab, enter the value of **Computational window H [Å]** equal to 2500 Å.

1.5. Click on the **Start** button to run the exposure simulation.

1.6. To review the calculated yield of scission, you can build plots as shown in Figure 38. Select **Tools/Plot** and load the yield of scission, then select **Plot/Plot2D/Plot XZ** and **Plot/Plot1D/Plot X 1D**.

Note 1.1: The described simulation can be relatively time consuming. To decrease the time of computation, user can either prepare a smaller input geometry file (for example, 40×40 pixels), or increase **Backscattering step size** in the **Parameters** tab.

[1] M.A. Mohammad et. al, (NINT and University of Alberta, 2012) to be published.

[2] M.A. Mohammad, K. Koshelev, T. Fito, D. Ai Zhi Zheng, M. Stepanova, and S. Dew, Jpn. J. Appl. Phys. 51 (2012) 06 FC05.

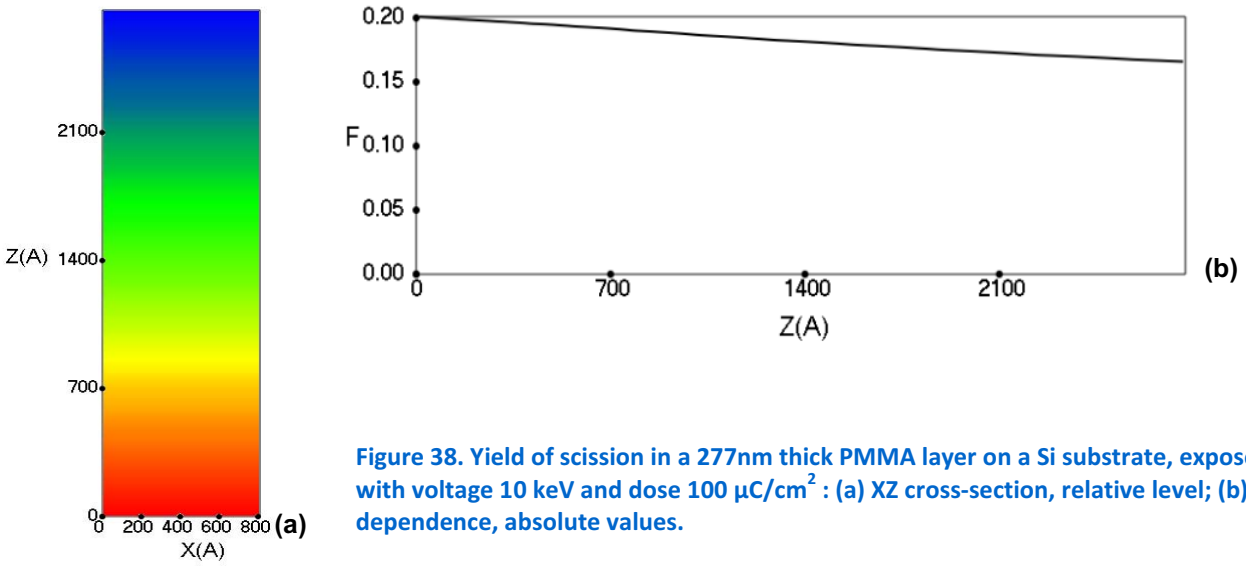


Figure 38. Yield of scission in a 277nm thick PMMA layer on a Si substrate, exposed with voltage 10 keV and dose 100 μC/cm^2 : (a) XZ cross-section, relative level; (b) Z dependence, absolute values.

2. Building a contrast curve for PMMA in MIBK:IPA 1:3 developer and 22°C

2.1. To build contrast curves, exposures must be simulated for several doses. To compute the yields of scission for different doses, use **Tools/Dose Convertor**. Make it sure that in the **In file** edit window, the scission yield file computed previously for the dose of 100 μC/cm^2 is selected. In the **Out path** edit window, specify the output file. Enter the factor of conversion 0.2 in the **Factor:** edit box and click on the **Convert** button (Figure 39). This will generate the distribution of the yields of scission for the dose 0.2×100 μC/cm^2 = 20 μC/cm^2. Repeat the conversion to produce a desired set of exposure doses, changing the names of corresponding scission yield files. In this example, the factors 0.20, 0.26, 0.32, 0.38, 0.44, 0.50, 0.56, 0.62, 0.68, 0.74, 0.80, 0.86 and 0.92 are employed to generate the doses of 20, 26, 32, 38, 44, 50, 56, 62, 68, 74, 80, 86 and 92 μC/cm^2, respectively.

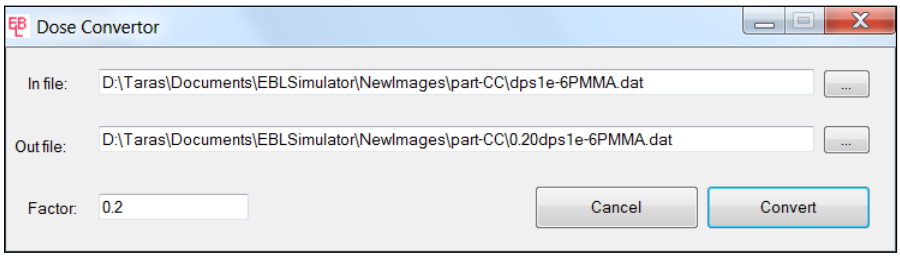


Figure 39. Using the distribution of the scission yield of for 20 μC/cm^2 dose from a 100 μC/cm^2 one.

2.2. To compute the development profiles, switch to the **Development** tab and check **Model 1.** Select **PMMA** resist and **MIBK:IPA** developer in the drop-down lists, enter temperature 22°C in the **Temperature dependence for β** block and click on the **Calculate β** button. Then enter development time of 20 seconds.

2.3. Click on the "**…**" button to load a proper scission yield file, and press **Start**. Indicate a file name to store the output.

2.4. Open **Tools/Plot** and load the computed development profile, then select **Plot/Plot2D/Plot XZ**. Use the mouse to move pointer to the polymer area (red color) and double click. Record the remaining resist thickness (denoted as **Z dimension**). In Figure 40, the remaining resist thickness is equal to 2390 Å. Find a ratio of this value with the initial resist thickness, (in this case, 239nm/277nm = 0.863).

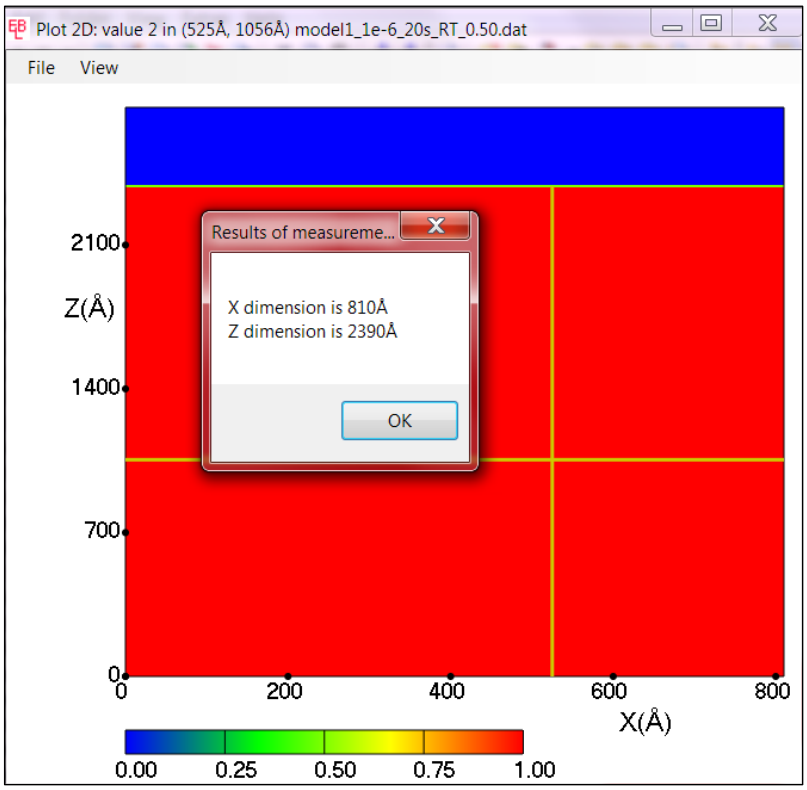


Figure 40. Remaining resist for an initially 277 nm thick PMMA layer on a Si substrate, exposed by 10 keV electrons with the dose of 50 μC/cm^2 and developed in MIBK:IPA 1:3 for 20 seconds at room temperature. In the plot, red color denotes remaining PMMA and blue color indicates clearance.

2.5. Repeat steps 2.3 and 2.4 for every distribution of the yield of scission from step 2.1 and plot the corresponding thickness ratios as a function of exposure dose. The resulting plot is shown by the solid line in Figure 41.

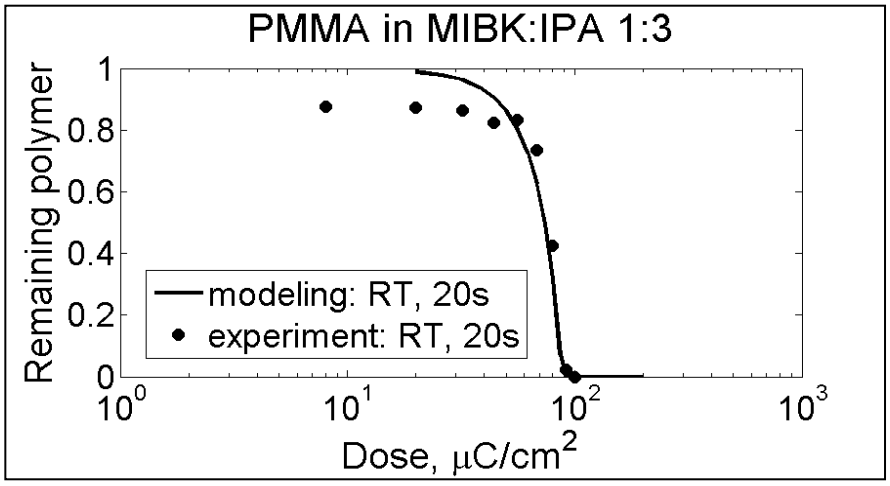


Figure 41. Simulated (line) and experimental[1] (points) contrast curves for PMMA resist exposed by 10 keV electrons and developed in MIBK:IPA 1:3 for 20 seconds at room temperature.

3. Contrast curve for PMMA in IPA:Water 7:3, 20 s development at -15°C

3.1. To generate the distribution of the yield of scission, repeat steps 1.2 – 1.5 choosing **Resist thickness** equal to 2720 Å to reproduce the experimental settings[1].

3.2. Use **Dose convertor** to generate the yield of scission distributions for exposure doses of 10, 60, 80, 100, 120, 140, 160, 180, 200, 220, 240, 260, 280, 300 and 500 μC/cm^2.

3.3. Switch to **Development** tab, check **Model 1**, in the **Developer** drop-down menu list select **IPA:Water 7:3**, in the **Temperature dependence for β** block enter temperature equal to –15°C, and click **Calculate β** button. Make sure that 20 s development time is entered.

3.4. Repeat steps 2.3 and 2.4 for all yield of scission distributions generated on step 3.2 and plot a contrast curve, see also solid line in Figure 42.

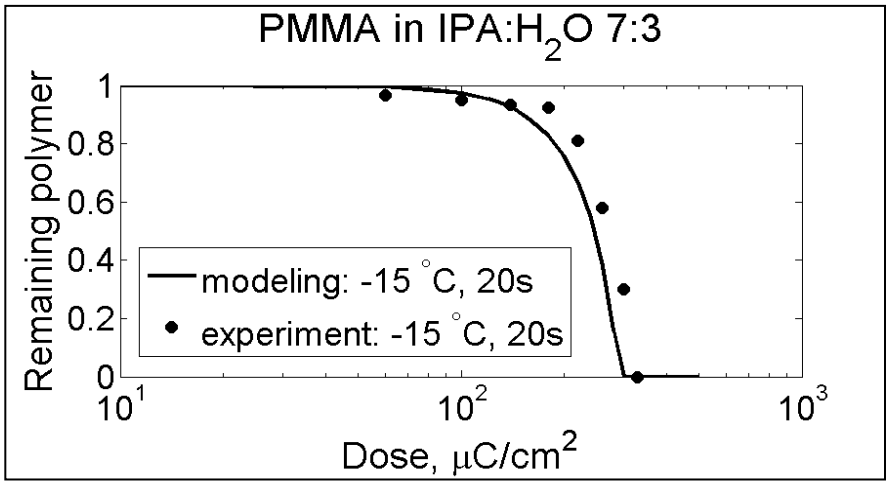


Figure 42. Simulated (line) and experimental[1] (points) contrast curves for PMMA resist exposed by 10 keV electrons and developed in IPA:water 7:3 mixture for 20 seconds at –15°C.

4. Contrast curve for ZEP in ZED-N50, 5 s development at 22°C

4.1. To generate the distribution of the yield of scission for ZEP, repeat steps 1.2 – 1.5 selecting ZEP in the **Resist** drop-down menu box and setting the **Resist thickness** equal to 2940 Å to reproduce experimental settings[1,2].

4.2. Use the **Dose convertor** to generate the yield of scission distributions for 1, 10, 16, 18, 20, 22, 24, 26, 28, 30, 32, 34, 36 and 50 μC/cm^2.

4.3. Switch to the **Development** tab, check **Model 1**, and select **ZEP** and **ZED-N50** in **Resist** and **Developer** drop-down menus, respectively. Enter temperature 22°C in **Temperature dependence for β** block, click the **Calculate β** button, and enter 5 seconds in the **Development time** box.

4.4. Repeat steps 2.3 and 2.4 for all scission yield distributions from step 4.2 and plot a contrast curve (solid line in Figure 43).

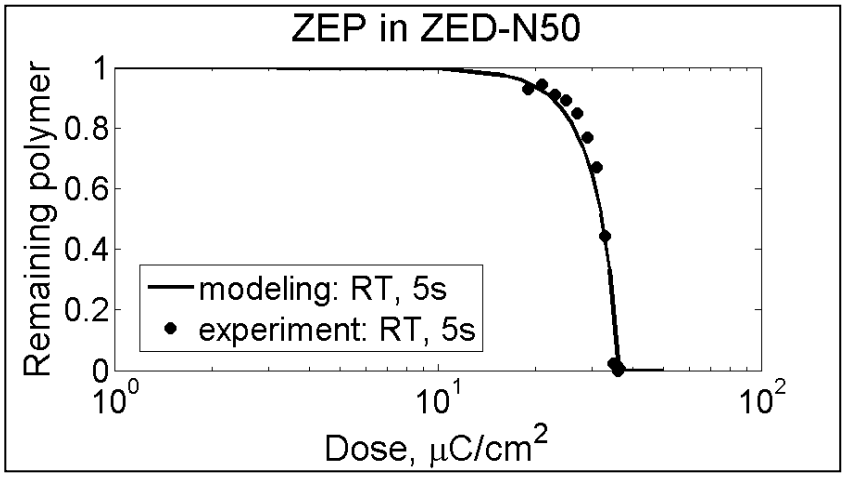


Figure 43. Simulated (line) and experimental[1,2] (points) contrast curves for ZEP 520 resist exposed by 10 keV electrons and developed in ZED-N50 mixture for 5 seconds at room temperature.

Note 4.1: If so desired, advanced users can employ their own experimental contrast curves for custom-tuning of development parameters to be entered in the **Development** tab. Such customized development parameters may be used as a first approximation to predict nanoscale features in PMMA or ZEP resists given that the developer and development temperature are the same as in the contrast curves from which the parameters have been extracted.

V. Modeling of Exposure with Conductive Layer

EBL Simulator supports inclusion of a conductive layer on top of a resist during exposure (Figure 44). Such conductive layers are employed as anti-charging solutions to avoid pattern damage by electrostatic charge in case if insulating substrates such as fused silica are used. [1] After exposure, conductive layers are removed. The simulator supports conductive polymer (Mitsubishi Rayon Co.), aluminum, or copper layers deposited on top of PMMA or ZEP resists on various substrates. The example below describes the steps used to model exposure and development of a periodic array of dots with a 50 nm pitch, in a 90 nm thick layer of PMMA on a fused silica substrate, covered by a 10 nm thick layer of aluminum using the EBL Simulator.

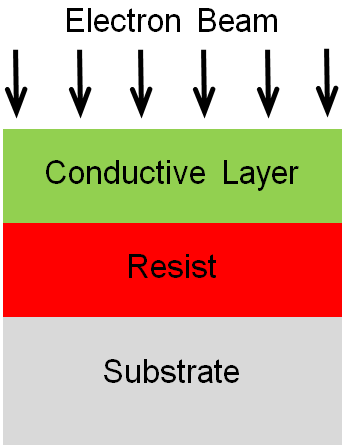


Figure 44. Scheme of EBL exposure with anti-charging conductive layer on top of a resist[1].

1. Example:
Exposure of PMMA resist with Al conductive layer on fused silica substrate

1.1. Prepare graphical file (BMP, TIF, or JPG) with size 50×50 pixels, which corresponds to a 50 nm × 50 nm area. Fill the entire area with black color and insert a white pixel in the center (Figure 45).

1.2. Launch the simulator. In the **Geometry** tab, check **Load from file**, load the graphical file, and check the **Periodic** checkbox to simulate a large periodic array of dots (Figure 46(a)).

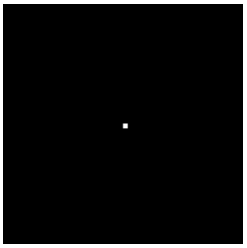


Figure 45. Exposure pattern for a periodic array of dots.

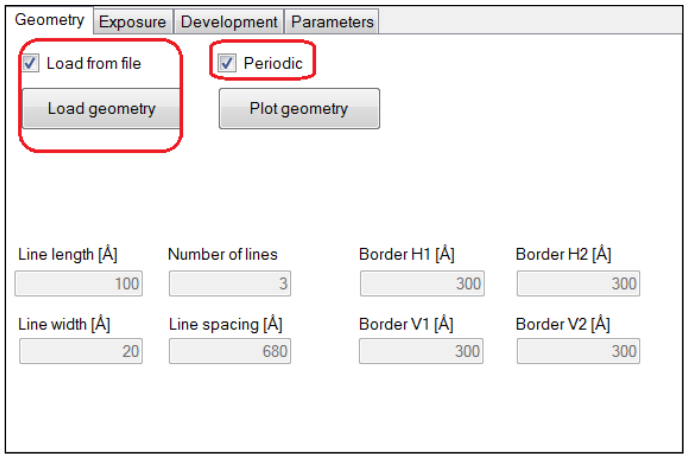
[1] M. Muhammad, S. C. Buswell, S. K. Dew and M. Stepanova, J. Vac. Sci. Technol. B 29 (2011) 06F304.

1.3. Switch to the **Exposure** tab (Figure 46(b)). Select **PMMA** in the **Resist** drop-down menu list and enter the value of **Resist thickness** equal to 900 Å. Select appropriate substrate in **Substrate** drop-down list (**Fused Silica** in this example) or otherwise press **Customize** and enter the average atomic number (10) and density (2.201 g/cm^3) of fused silica[2] [3] in the **Average substrate Z** and **Substrate density** edit boxes, respectively.

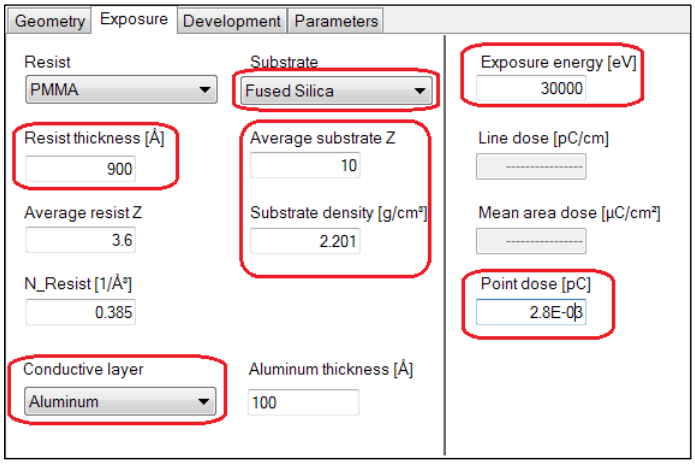
1.4. In the **Conductive layer** drop-down menu list choose **Aluminum**. This will activate the conductive layer thickness edit box, in which a thickness of 100 Å should be entered.

1.5. Set **Exposure energy** equal to 30000 eV. In the **Point dose** control box, enter "2.8E-3", which corresponds to dose of $2.8 \cdot 10^{-3}$ pC/dot, or 2.8 fC/dot (Figure 46 (b)).

1.6. Since the resist layer is relatively thick, the computational window in the **Parameters** tab needs to be increased (see **Help** for the definition of this parameter). In **Parameters** tab, enter the value of **Computational window H [Å]** equal to 2500 Å.



(a)



(b)

Figure 46. (a) - Geometry tab; (b) - Exposure tab.

[2] Average atomic number of SiO_2 is $\frac{14 + 2 \cdot 8}{3}$ =10.

[3] http://www.sciner.com/Opticsland/FS.htm

1.7. Click the **Start** button. This will initiate simulation of the 3D distribution of the yield of scission in the resist with accounting for the widening of the electron beam due to elastic scattering in the conductive layer.

1.8. To plot the distribution of the yield of scission, select **Tools/Plot** and load the file. Select **Plot/Plot2D/Plot XZ** (Figure 47) or a different plotting option as desired.

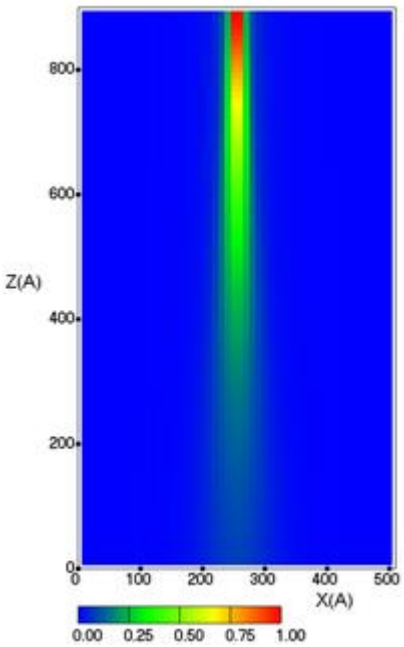


Figure 47.
Cross-sectional view of the distribution of the yield of scission in PMMA on fused silica substrate, coated with a 10 nm thick layer of aluminum (steps 1.1 – 1.8). The Al layer and the substrate are not shown.

Note 1.1: Plots of scission yield distributions and other simulation outputs are generated for the resist only. The conductive layer does not appear in the plots.

Note 1.2: Inelastic collision energy losses of electrons in thin conductive layers are considered minor and not accounted for in the present version of the simulator.

Note 1.3: The simulator accounts for widening of the electron beam due to elastic scattering in the conductive layers. The widening is determined by the transport mean free path[4] of electrons in the layer, and depends on the layer thickness. Material parameters employed to determine the transport mean free paths are listed in Table 3.

Table 3. Material parameters employed to simulate electron beam widening in conductive layers.

Material	Average atomic number	Average atomic weight	Density, g/cm^3
Conductive polymer	5.33	10.34	1.0
Al	13	26.98	2.7
Cu	29	63.55	8.94

[4] D. Liljequist, F. Salvat, R. Mayol, and J. D. Martinez, J. Appl. Phys. 65 (1989) 2431.

2. Development profile generation

As long as conductive layer is removed after exposure, simulation of development is not different from bare resist development. In this example, a 10 s development in IPA:Water 7:3 mixture at 22°C is simulated for the exposure pattern obtained by steps 1.1-1.7. If changing the temperature, click the **Calculate β** button to update the β value for the selected temperature.

2.1. Switch to the **Development** tab and check **Model 1**. Make it sure that the development conditions are set as in Figure 48, click **Start** and choose a file to store the output.

2.2. Plot the output, for example as shown in Figure 49.

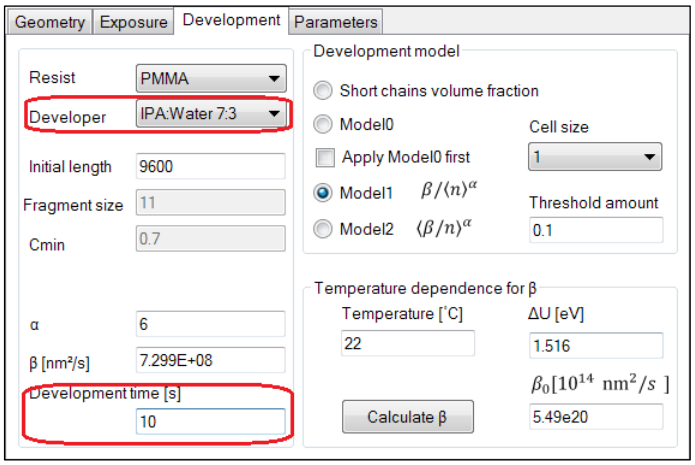
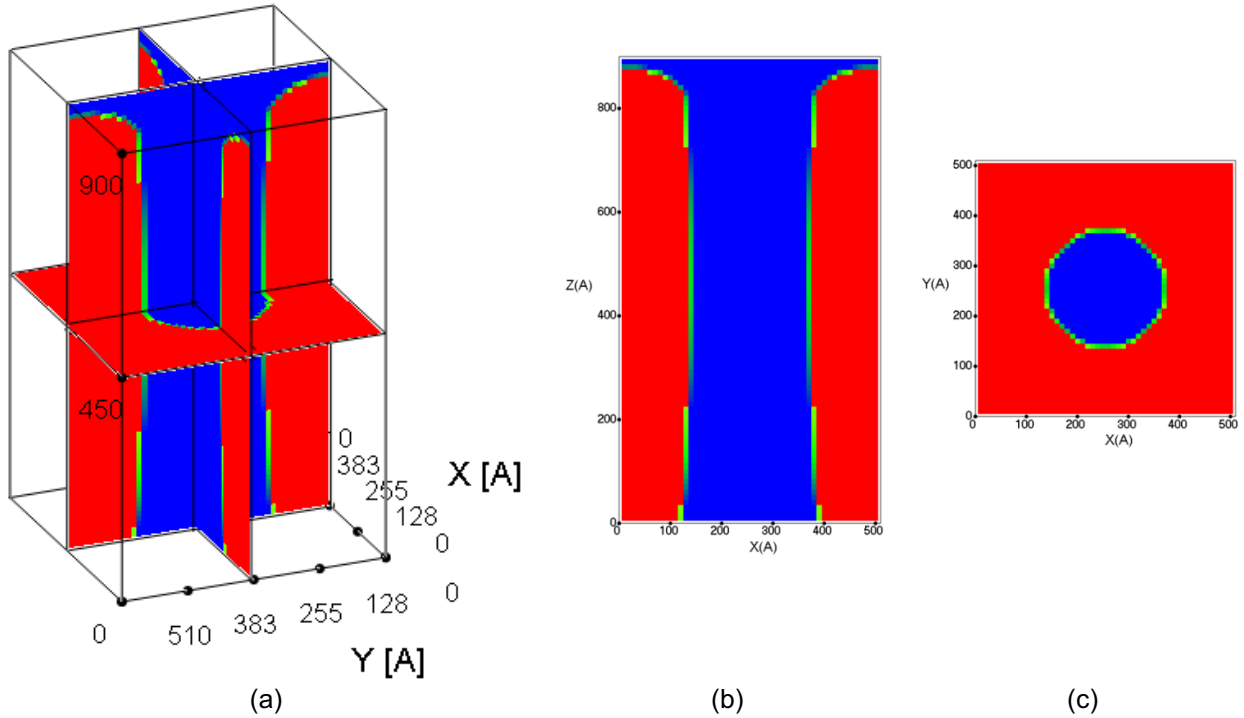


Figure 48. Development tab settings.



(a) (b) (c)

Figure 49. Developed profiles of PMMA exposed with a 10 nm thick aluminum layer: (a) – general 3D view; (b) – XZ cross-section; (c) – XY cross-section.