EXCALIBUR: A Monte Carlo Simulation for the Design of Lithographic Resists

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Developing new resist materials for electron beam and ion beam lithography requires knowledge of the interactions of the electrons and ions in the resist to predict the lithographic process. To this end, a Monte Carlo Simulation named 'EXposure CALculations with Ion Beams to Understand Resists' (EXCALIBUR) was developed to simulate resist candidates for investigation, prior to synthesis, to streamline the time expensive process of manufacturing and characterising new resist materials.

The EXCALIBUR simulation led us to develop a new class of ultra-high dry etch selectively ion and electron beam resist which is based on a family of heterometallic rings (Figure 1)[1,2]. The ion beam resist was simulated using 35 keV Helium ions and showed that a resolution of 8 nm half pitch could be achieved (Figure 2a). Ion beam lithography experiments demonstrated that the negative tone resist has attained a high resolution of 8 nm half pitch while exhibiting a sensitivity of 22 pC/cm (Figure 2b). The incident ions (seen in Figure 2a) appear to hide the extent of the total exposure contribution made by the secondary electrons (SE) and back scattered electrons (BSE). Therefore, we have taken the SE and BSE and superimposed the ion trajectories directly on top of the SEM image shown in Figure 2b. Figure 2c shows that the exposure mechanism is from BSE, this is because the resist thickness is 5 nm, hence, the majority of the low energy (< 30 eV) ion interaction occurs within the silicon (incident Helium ion energy is 35 keV), thus producing BSE in the immediate exposure area (Figure 2d). It was determined by the simulation that the total number of BSE's generated in resist was 629 per spot and exposes the resist from the back side of the resist. This work illustrates a strong agreement between the simulation and the experimental results.

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[1] S. M. Lewis et al., *Nano Lett.* **19**(9), 6043–6048 (2019)

[2] S. M. Lewis et al., *Angew. Chem. Int. Ed.*, **56**, 6749 (2017)

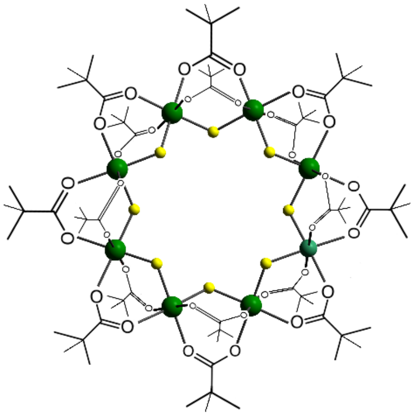

Figure 1: a) $Cr_8F_8(Pivalate)_{16}$. The structure of the molecules in a crystal, in ball-and-stick representation. Cr atoms are green, F atoms are yellow. H atoms are omitted for clarity.

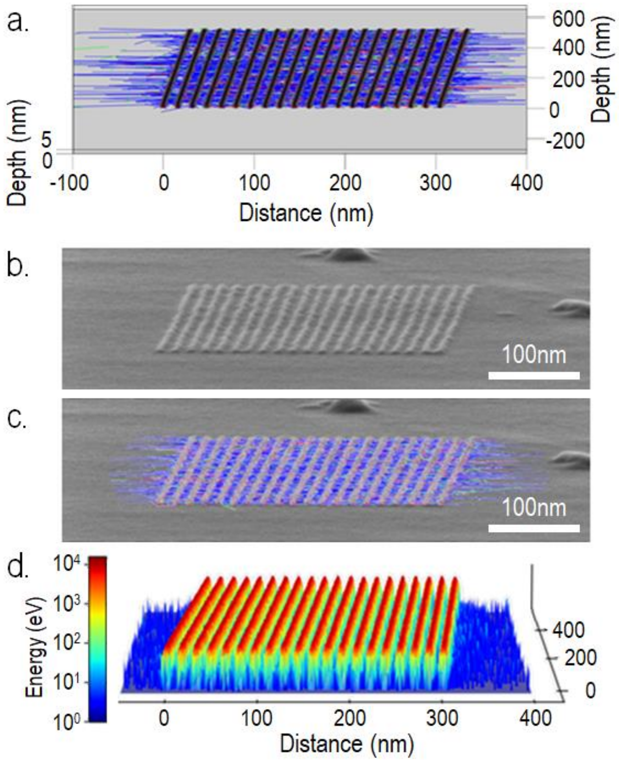

Figure 2: (a) 3D simulated tracks of Incident Ions (Black) and subsequent generations of secondary electrons (I:Red, II:Blue, III:Green and IV: Magenta) generated using EXCALIBUR. (b) Helium Ion micrograph of 16 nm pitch Helium ion beam lithography (HIBL) structures in $Cr_8F_8(Pivalate)_{16}$ resist on a silicon substrate[1]. (c) The same micrograph as b with a 3D simulation of ion and electron trajectories overlaid. (d) Energy deposit plot showing where energy is deposited in the x-y plane during HIBL exposure.