Monte-Carlo Simulations of Ion Beam Sputtering in Compounds

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An updated experimental and simulation based study of the evolution of nanostructures resulting from ion beam sputtering will be presented. The EnvizION Monte-Carlo based code was updated to simulate the sputtering process for a variety of ion beams and target compositions and structures. With the improved algorithm, the computational efficiency of this code permits the simulation of more detailed physics in larger scale problems where the doses involve millions of ions. In particular, the dynamic and cumulative sub-surface defects that occur during milling are tracked and an algorithm to dynamically minimize surface energy at the evolving nanostructure interface was implemented. The power of the simulation is studying the dynamic development of nanoscale focused ion milling in elemental and multi-component targets, where the resulting structures may be high aspect ratio both in plane and out of plane. The effect of target composition and ion species on the resolution of focused ion beam induced sputtering of nanostructures were explored. The dose-dependent sputter yields and backscattered ion trajectories were analyzed. Targets composed of SiO_2 were found to exhibit preferential sputtering of oxygen, affecting the near surface composition dynamically as a function of the dose.

In this presentation, we describe the novel features of the Monte-Carlo simulation code base, and will compare simulation and experimental results of various targets (Cu, Si, SiO_2) and ions (Ne^+, Ga^+). The significance of the near surface structural and compositional changes and defects such as vacancies and interstitial atoms on the formation of the etched vias will be addressed.

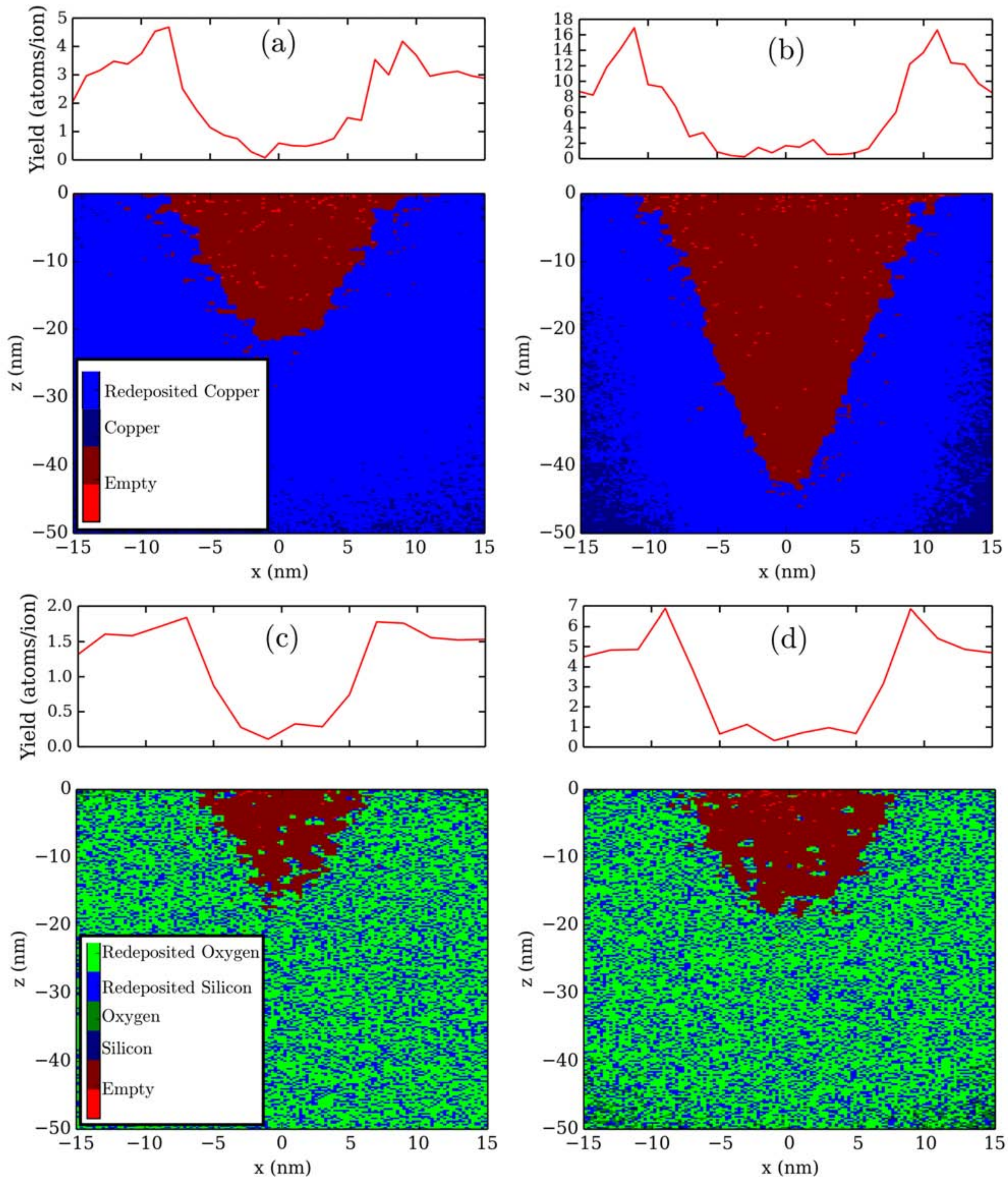

Figure 1: Cross section of three dimensional nanostructures, nanomachined by a 20 keV beam with a 10 nm full width at half maximum (FWHM) Gaussian profile at a constant dose of 10^{23} ions/cm^2. The plots show the sputter yield as a function of the x-coordinate of the corresponding cross section: (a) Ne^+ ion beam, copper target, (b) Ga^+ ion beam, copper target, (c) Ne^+ ion beam, SiO_2 target, and (d) Ga^+ ion beam, SiO_2 target.