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Nanoscale mechanics of focused ion beam processing

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ABSTRACT

Focused ion beam (FIB) processing is a widely used microscopic material removal method with precise dimensional control, for applications ranging from electron microscope sample preparation to DNA sequencing nanopore processing. Despite the widespread use of FIB, the basic material removal mechanisms are not well understood. In this study we present the first complete atomistic computational studies of high-flux FIB. We use large-scale parallel molecular dynamics simulations to study nanopore fabrication in freestanding thin film targets. Our simulations consider up to 5.1 million atoms, for durations of up to millions of time steps. We focus on understanding two key nanoscale mechanics phenomena that emerge from the large scale MD simulations of FIB: the role of explosive boiling as a material removal mechanism, and the role of Marangoni effects in the mixing and transport that occur at the atomic scale. Nanopore fabrication using FIB is typically understood to occur via sputter erosion. It is thought that, on average, each ion impact sputters two or three target atoms from a typical freestanding silicon specimen, thinning the target, and eventually forming a through-thickness nanopore. Although this theory may work for low-flux systems, where individual ion impacts are sufficiently separated in time that it is possible to consider them as independent events, it cannot explain the thermal events observed during high flux simulations. Our detailed molecular dynamics simulations suggest that for ion beam fluxes above a threshold level, the dominant mechanism of material removal changes to a significantly accelerated, thermally dominated process. During this time, the target is heated faster than it cools via thermal conduction, leading to melting, with local temperatures approaching the critical temperature. This leads to explosive boiling of the target material, as identified by the violent phase change occurring in the rapidly heated liquid. Spontaneous bubble formation occurs because of large fluctuations of density in a very small volume. Atomic mass is rapidly rearranged via bubble growth and coalescence, leading to a material removal process order of magnitude faster than would occur by sputter erosion. When a high flux FIB process is tightly focused on a silicon target, as in the case of nanopore formation, a large temperature gradient gives rise to a circulating flow of liquid silicon because of steep surface tension gradients – or a Marangoni flow. This drives mass transfer inside the target and along the newly created nanopore surfaces, from regions of high temperature to regions of low temperature. For films of a particular thickness, two counter-circulating atomic scale flow regions form in the target. Thus, the Marangoni flow phenomenon drives mass transfer and material rearrangement at the top and bottom free surfaces.