ATOMISTIC ORIGINS OF THE SPUTTER EROSION SURFACE INSTABILITY

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Ion-bombardment is a widely used microelectronics processing tool, and it is expected to be an important fabrication tool for nanotechnology. In this energetic process, the target material, often a semiconductor such as silicon, is significantly affected mechanically by the incident ion irradiation. Under certain ion-bombardment conditions, the spontaneous formation of nanoscale ripples and dots is observed. The instability yields reproducible, uniform, ordered arrays of nanostructures, including either well defined lines or dots that may be useful in nanoelectronics, optoelectronics, or nanomechanical applications requiring surface patterning. Until now, only phenomenological continuum models have been used to interpret the widely seen experimental results, and no models have achieved the predictive ability needed to shed light on the basic physics and mechanics or to guide the process for use as a potential nanomanufacturing method. Molecular dynamics (MD) simulations are used in the present work to fully investigate the mechanisms behind the process. The results of the MD studies are interpreted spatially and temporally over many orders of magnitude so that the atomistic results can be linked to continuum experimental observations.

In the present work, the molecular dynamics simulations are used together with both linear stability analysis and continuum surface evolution models to uncover the atomistic origins of the sputter erosion surface instability. A large database of molecular dynamics results as a function of variables including temperature, stress, incident angle, energy, and surface characteristics is collected; the results are then incorporated into continuum models. The studies reveal the atomistic mechanisms by which medium energy ions incident on an initially flat surface preferentially amplify surface roughness, even as thermally activated mass transport tends to smoothen surfaces out to longer length scale features. Numerous possible stabilizing and ordering mechanisms occurring at the atomistic scale are considered including viscous relaxation, sputtered atom redeposition, and other short time scale correlations between change in surface height and spatial derivatives of the local surface morphology.

The key conclusion of the study is that existing models fail to include the effects of mass redistribution due to individual ion impacts. In the context of the existing theoretical understanding of sputter ripple formation, the mass redistribution results in a sub-nanometer scale pileup region near each individual ion impact site. This subtle, local feature, which is too small to directly image experimentally, leads to significant long range effects, such as the experimentally observed saturation in ripple amplitudes that occurs after extended sputter erosion of a surface. Two-dimensional and three-dimensional computational results are presented to illustrate these points, and to show the strong agreement with available experimental data.

Keywords: Surface instability, molecular dynamics, semiconductor