MECHANICS OF ION-BOMBARDMENT INDUCED INSTABILITY OF SEMICONDUCTOR SURFACES

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Summary Semiconductor surfaces exposed to low energy ion bombardment are unstable with respect to formation of submicron-scale ripples and dots. This phenomenon is widely understood to be due to a competition between surface roughening due to erosive and mass rearrangement effects, and surface smoothing due to diffusive effects. However, the proposed mechanisms for these instabilities have yet to explain the rich range of patterns that are observed experimentally. Here we show that smoothing balanced by impact angle dependent mass redistribution explains the atomistic origin of ripple formation and orientation, particularly angle dependent transitions between different orientations. We develop a multiscale atomistic-to-continuum computational model that generates surface morphology results consistent with experimental observations for a range of ions, ion energies, and target materials.

INTRODUCTION

Irradiation of initially smooth surfaces by keV ions is widely known to cause formation of periodic ripples and dots, with wavelengths on the order of 100-1000nm and amplitudes on the order of 10nm. Silicon surfaces under Ar+ ion bombardment have been the most widely studied case, but other ions (Xe, Kr, etc.) have been found to cause ripple formation on surfaces as widely varying as semiconductors, metals, and insulators.[1-6] This phenomenon has been studied experimentally, but a simple theoretical model due to Bradley and Harper,[7] invoking assumptions about the ion energy deposition in the target material due to Sigmund,[8] has formed the basis for the conventional understanding. The central idea in this theory is that sputter-induced erosion roughens a surface, while diffusion smooths the surface, and the competition leads to the emergence of a dominant surface wavelength. The erosion, in particular, is thought to depend in a simple, linear way on the deposition of energy on the surface by incident ions.

In our previous work, we showed that it is not erosion that roughens the surface, but rather rearrangement of mass near the surface that dominates the development of surface morphology.[9] We connected this observation to the concept of an individual-ion response function called the crater function.[10] Then, by computing statistically averaged crater functions representative of individual ion impacts, we were able to show numerically the formation of surface morphology through the use of a multiscale, coupled atomistic/continuum modelling method. In the present work, we first investigate the relationship between ion energy deposition in the target material and the associated sputtering behaviour. This work is based on careful interpretation and statistical analysis of molecular dynamics results. We then consider the relationship between the geometry of the angle dependent crater functions and the orientation of the ripples that form on the surface.[11]

ION ENERGY DISTRIBUTION IN THE TARGET

Using molecular dynamics (MD) simulations of individual ion impacts (Ar, Xe, Kr, or Ra), we determine the spatial distribution of energy deposited in ion-bombarded silicon and germanium targets. The details of the MD calculations are reported elsewhere.[9-11] We characterize the shape of the locally energized region around the time at which sputtering takes place. As shown in Figure 1, the region of energy deposition is approximately ellipsoidal for near normal incidence, but significantly different at grazing incidence.[12] The normal incidence energy distribution, in particular, is very well matched to the distribution hypothesized by Sigmund, and parameterized by lengths α, α_2, β_1,

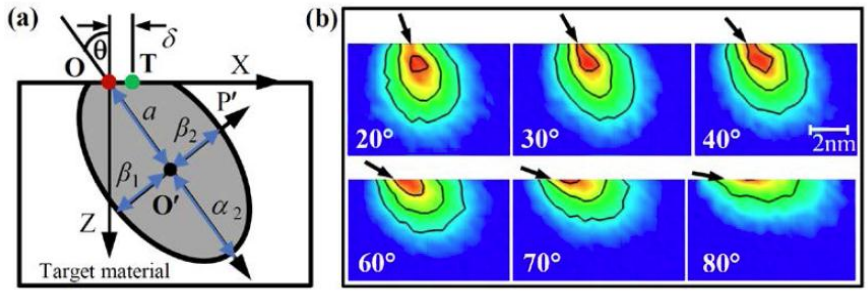

Figure 1: Characterizing the shape of the ion-impact energy distribution in the target.[12] At near normal incidence, the energy distribution is nearly ellipsoidal, as predicted by Sigmund.

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and β_2. The relationship between sputtering and local energy deposition, however, is significantly nonlinear and time-dependent. This observation contradicts the simple hypothesis of Sigmund, and has important implications for the theories of surface evolution based on Sigmund's description.

EFFECT OF IMPACT CRATER ASYMMETRY ON SURFACE RIPPLE STRUCTURE

Using similar MD simulations, in this case to determine the local surface height change near the impact of an individual ion, we determine a statistically averaged crater function whose shape depends on angle of incidence, ion energy, and ion/target material combination.[10] We then compute several scalar spatial moments of the crater function that describe the balance of the material rearrangement upstream and downstream from the point of impact. These moments can be correlated with a prediction of the orientation of ripples expected to form on the surface. For a particular ion/target material combination, such as Ar/Si, we can then form a phase diagram of ripple orientation as a function of ion energy and angle of incidence, as shown in Figure 2. Our predictions, the details of which are reported in another article,[11] are in excellent agreement with experiments in the literature.

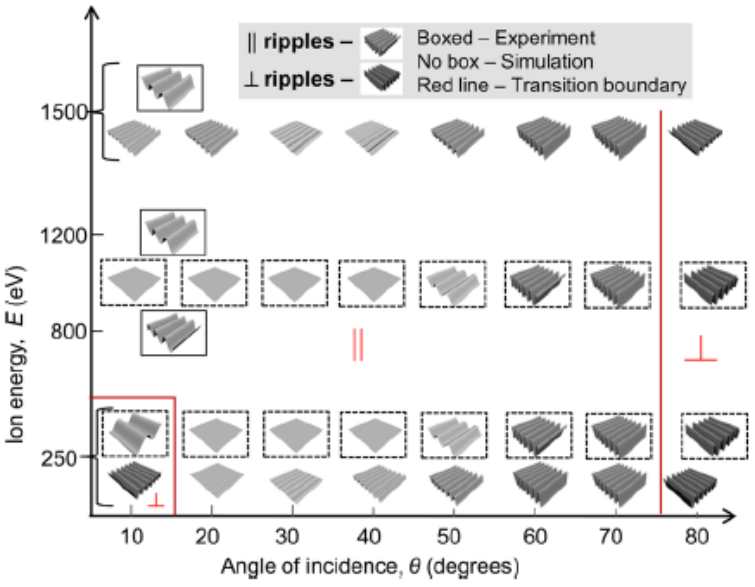

Figure 2: Phase diagram of predicted surface ripple orientation relative to ion beam direction, as a function of angle of incidence and ion energy. The predictions based on molecular dynamics results are in good agreement with experiments. Figure is reproduced from Reference 11.

CONCLUSIONS

We show through careful statistical analysis of molecular dynamics results for individual ion impact events on semiconductor surfaces that (i) the geometrical distribution of energy in the target material is ellipsoidal, as hypothesized by Sigmund, but the relationship between energy and sputtering is nonlinear and time-dependent, contrary to the conventional view; and, (ii) the geometrical features of the individual ion crater function can be used to accurately predict the orientation of surface ripples, which occur over much longer length and time scales. Both key conclusions are consistent with experimental data in the literature.

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