Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

A multi-scale model using single ion impacts predicts large-scale pattern formation in irradiated solids SCOTT NORRIS, Southern Methodist University — Energetic particle irradiation of solids can lead to highly regular nanoscale pattern formation under the right environmental conditions. The widespread use of this technology in current industrial settings for doping and hardening suggests the promise of harnessing spontaneous pattern formation to create novel devices. However, existing theoretical models of ion irradiation fail to agree broadly with experiment even in the linear regime of small-amplitude patterns. A central challenge in modeling this system is to rigorously connect the pico-second effect of single ion impacts, spanning mere nanometers of materal, to the long-time evolution of surface structures spanning tens to hundreds of nanometers. Here, we present a multi-scale framework that achieves this end. We start with molecular dynamics simulations of single ion impacts, and upscale this data into a continuum PDE for the surface topography. Stability analysis of the PDE predicts the characteristic pattern wavelength as the incidence angle is varied. The predictions agree remarkably well with experiment, and overturn the long-held assumption that pattern formation is due to the removal of target atoms by sputter erosion.

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Date submitted: 29 Nov 2011 Electronic form version 1.4