Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Entropic Influence on the Aggregation Physics of Interstitial Point Defects in Silicon TALID SINNO, SUMEET KAPUR, ALEX NIEVES, University of Pennsylvania — The evolution of self-interstitials and their aggregates during the annealing of ion-implanted silicon has received a tremendous amount of attention because of their strong, non-linear effects on the diffusion of dopants. The implantation process leads to extensive lattice damage, which must be healed by thermal annealing. Also generated by the implantation process is a large number of self-interstitials which lead to enhanced dopant diffusion during annealing known as Transient Enhanced Diffusion, or TED. A major obstacle to understanding and quantitatively predicting TED is the formation of a variety of self-interstitial aggregates, which range from small amorphous three-dimensional clusters, to planar stacking-faults with various crystallographic orientations. In the present study, we use large-scale constant-stress MD simulations to dynamically simulate the evolution of an ensemble of highly supersaturated self-interstitials at various temperatures and pressures. We show that the simulated interstitial clustering into various types of planar structures exhibits a complex thermodynamic-kinetic phase diagram that is sensitively controlled by entropic factors. The observations are studied with a recently developed approach that maps out the potential energy landscape in the vicinity of the defect cluster and allows for the total (classical) free energy to be analyzed.

Talid Sinno
University of Pennsylvania

Date submitted: 03 Jan 2011 Electronic form version 1.4