

Abstract Submitted  
for the MAR13 Meeting of  
The American Physical Society

**Study of the diffusion of points defects in crystalline silicon using the kinetic ART method** MICKAEL TROCHET, Université de Montreal, PETER BROMMER, University of Warwick, LAURENT-KARIM BELAND, JEAN-FRANCOIS JOLY, NORMAND MOUSSEAU, Université de Montreal — Because of the long-time scale involved, the activated diffusion of point defects is often studied in standard molecular dynamics at high temperatures only, making it more difficult to characterize complex diffusion mechanisms. Here, we turn to the study of point defect diffusion in crystalline silicon using kinetic ART (kART)[1-2], an off-lattice kinetic Monte Carlo method with on-the-fly catalog building based on the activation-relaxation technique (ART nouveau). By generating catalogs of diffusion mechanisms and fully incorporating elastic and off-lattice effects, kART is a unique tool for characterizing this problem. More precisely, using kART with the standard Stillinger-Weber potential we consider the evolution of crystalline cells with 1 to 4 vacancies and 1 to 4 interstitials at various temperatures and to provide a detailed picture of both the atomistic diffusion mechanisms and overall kinetics in addition to identifying special configurations such as a 2-interstitial super-diffuser.

[1] F. El-Mellouhi, N. Mousseau and L.J. Lewis, Phys. Rev. B. 78, 153202 (2008)

[2] L. K. Béland, P. Brommer, F. El-Mellouhi, J.-F. Joly and N. Mousseau, Phys. Rev. E 84, 046704 (2011).

Mickael Trochet  
Université de Montreal

Date submitted: 04 Jan 2013

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