A computational atomistic study of the relaxation of ion-bombarded c-Si on experimental time-scales: an application of the kinetic Activation Relaxation Technique

LAURENT KARIM BÉLAND, NORMAND MOUSSEAU, Dept. de physique and RQMP, Universite de Montreal, Canada — The kinetic activation relaxation technique (kinetic ART) method, an off-lattice, self-learning kinetic Monte Carlo (KMC) algorithm with on-the-fly event search,\(^1\) is used to study the relaxation of c-Si after Si\(^-\) bombardment at 3 keV. We describe the evolution of the damaged areas at room-temperature and above for periods of the order of seconds, treating long-range elastic deformations exactly. We assess the stability of the nanoscale structures formed by the damage cascade and the mechanisms that govern post-implantation annealing.