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**Accelerated Kinetic Monte Carlo Simulations of Vacancy-Mediated Arsenic Diffusion and Clustering in Silicon** BRIAN PUCHALA, University of Michigan, MICHAEL FALK, Johns Hopkins University, KRISHNA GARIKIPATI, University of Michigan — During semiconductor device fabrication, ion implantation of dopants creates large populations of defects, vacancies and interstitials, which mediate dopant diffusion. Experiments have shown large changes in dopant diffusivity in silicon as a function of annealing time and dopant concentration. We perform kinetic Monte Carlo (KMC) simulations of vacancy-mediated arsenic diffusion in silicon to investigate the effect of dopant concentration, distribution and clustering on diffusivity. In order to follow the diffusion and breakup of clusters, on the order of minutes, our KMC simulations are accelerated using absorbing Markov chain analysis on states intelligently chosen on-the-fly to fill trapping basins in the local energy landscape. At lower dopant concentrations, we calculate the diffusivity and breakup rates of different cluster types and a mean field approach can be used to describe the overall cluster population evolution and dopant diffusivity. Above a critical concentration this mean field description fails as dopants become close enough to form a percolating structure throughout the material. At all concentrations, diffusivity decreases significantly over time as larger, less mobile clusters form.

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