

565b On-Lattice Kinetic Monte Carlo Simulations of Point Defect Aggregation in Entropically Influenced Crystalline Systems

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An on-lattice Kinetic Monte Carlo (KMC) model for vacancy aggregation in crystalline silicon is presented. The process of vacancy aggregation during silicon crystal growth and wafer thermal annealing is technologically important because it leads to microscopic voids that are detrimental to microelectronic device yields and reliability in polished wafers. The KMC rate database is defined using a bond counting approach with extended interactions (up to the 8th neighbor shell). The bond energies are computed using a global regression approach in which the KMC model output is compared to two types of molecular dynamics-generated data: (1) the evolution of the cluster size distribution as a function of time (non-equilibrium data), and (2) the probability distribution function of local minima for single cluster configurations (equilibrium data).

Both approaches are shown to give consistent KMC models of the vacancy aggregation process only if the full interaction distance is included. The effect of the interaction distance on the aggregation dynamics and cluster morphology is probed using a series of numerical experiments. We show that standard on-lattice KMC models of point defect aggregation in crystals can severely underestimate configurational entropic contributions at high temperature because they fail to account for the presence of mechanically stable off-lattice configurations. Finally, we demonstrate how the present approaches circumvent this problem and suggest ways for coarse-graining off-lattice physics into lattice KMC models.