Simulation of Epitaxial Regrowth of Doped Silicon

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We conducted molecular dynamics (MD) simulations of solid phase epitaxial growth of As-doped Si using a modified Tersoff potential characterized via comparison to density functional theory (DFT) calculations, including energies of AsnV clusters. The Si:As systems were initialized by amorphizing the surface region of crystalline silicon via Si ion implantation. The remaining crystalline region provides dual function of controlling temperature in system without perturbing regrowth and providing seed for recrystallization. After recrystallization, isolated As atoms occupy substitutional sites, with the average number of nearest neighbors for As changing from about 3.3 in amorphous Si to 4 after crystallization. We observe V incorporation associated with high As concentrations, primarily at sites with multiple As neighbors. These observations are consistent with our previous model developed to explain kinetics of As shallow junction formation which assumed V incorporation at sites with 2 or more As nearest neighbors to account for experimental data.