COUPLING CONTINUUM ELASTICITY AND MASS TRANSPORT VIA ATOMISTIC MODELING: STRESS EFFECTS ON VACANCIES IN STILLINGER-WEBER SILICON

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Vacancies in silicon undergo an elastic relaxation that contributes to the formation energy of the defect. This elastic relaxation can also couple the defect energy to an externally applied elastic field causing changes in diffusivity and providing a driving force for molecular transport. Understanding this coupling is important for modeling the ways in which stress driven diffusive transport can control the growth of defects and distribution of dopants in semiconductors. We have performed molecular dynamics (MD) calculations of the relaxation and coupling in Stillinger-Weber silicon. Comparisons were made between these atomistic results and Green's function solutions of the elastic relaxation around a generalized force dipole. In these comparisons the boundary conditions of the elastic calculation were extracted directly from the MD simulation rather than by fitting the long-range elastic behavior. The formation energy and symmetry is observed to change under hydrostatic and shear loadings. We compare the strain field predicted by continuum mechanics methods directly to the atomistic results. We will discuss the important role of simulation cell geometry and system size in such atomistic/ continuum modeling.