KANZAKI FORCE AND FORMATION ENERGY OF LATTICE DEFECTS IN SI/GE(001) QUANTUM WELLS

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Kanzaki force and formation energy are basic properties of lattice (point) defects as related to experimentally measurable quantities, such as relaxation volume, surface stress and diffusion coefficient. In bulk matrices their calculation has been standardized either within the framework of first-principles calculations or within the lattice theory based on empirical interatomic potentials. However, it has been a long-standing difficulty in the presence of extended defects, such as surface and interface in advanced material systems. It poses a great challenge involving multiple length scales from atomic spacing to nanometers to continuum. In the present study, we have developed a Green's function (GF) based multiscale modeling of lattice defects in a trimaterial system and applied it to calculate the Kanzaki force and formation energy of lattice defects in Si/Ge quantum wells. The continuum and lattice GFs of trimaterials are used to seamlessly link the different length scales. Nonlinear behavior in the core of lattice defects is taken into account in an iterative scheme. We have examined a variety of point defects including vacancies and substitutions. It is found that when the Si/Ge matrices are strained as in their quantum-well state, their overall elastic property and the property of embedded defects change considerably from those in the unstrained state. In the strained Ge matrix the surrounding atoms may displace inwards or outwards from the site of a vacancy depending on the magnitude of straining in the matrix, showing a bifurcation phenomenon of structural phase transition. In the Si/Ge quantum-well structures, the defect properties vary sharply across the abrupt interfaces, as expected. The transition normally completes over a distance from two to four lattice constants depending on defect species. There appears to be little nonlinear effect in those defects except in C substitution due to its strong alternation to local bonding lengths.

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