

Using Large-Scale Simulations to Advance Understanding of Defects in Silicon

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Motivation—When the Sandia Pulsed Reactor (SPR-III) is decommissioned in 2006, a considerable gap will exist between the threat environment for which electronic components in nuclear weapons must be qualified and available testing environments. To bridge this gap, the Qualification Alternatives to the Sandia Pulsed Reactor (QASPR) program is developing new modeling capabilities that will be used in concert with experiments to qualify weapons. The goals of the QASPR program are ambitious in that the response of complicated circuits to neutron and gamma irradiation must be accurately predicted at short time scales. This requires, among other things, a thorough scientific understanding of the behavior of the defects generated in silicon (Si) devices during neutron irradiation.

Accomplishment—We have used density-functional theory to compute the energy levels and diffusion activation energies of the silicon vacancy and self-interstitial. In the calculations, periodic boundary conditions are applied to a supercell containing a defect surrounded by bulk material, effectively producing an infinite, periodic array of defects. The use of periodic boundary conditions yields an efficient computational scheme, however it also introduces spurious electrostatic and strain interactions, between the defect and its periodic replicas, which are difficult to quantify and may vary significantly with the size of the supercell. To remove these spurious interactions, we perform calculations in three different sized supercells and extrapolate the results to an infinite sized supercell. The calculations are performed in nominal 216-, 512-, and 1000-atom supercells and the results are then fit to the equation

$$E^f [D^q; L] = E^f [D^q; L \rightarrow \infty] - \frac{\alpha q^2}{\epsilon L} + \frac{A_3}{L^3} \quad (1)$$

where $E^f [D^q; L]$ is the formation energy of defect D^q in the supercell with length L , $E^f [D^q; L \rightarrow \infty]$ is the formation energy in an infinite sized supercell (determined from the fit), α is a Madelung constant, ϵ is the static dielectric constant of Si, and A_3 is the coefficient determined from the fit.

The fits of the supercell data to Eqn. 1 are very good as illustrated in Fig. 1. We have also examined how the results depended on two different forms of exchange and correlation; the local-density approximation (LDA) and the generalized-gradient approximation (GGA). In agreement with experimental results, the GGA yields a vacancy configuration with C_{2v} symmetry in the -1 charge state, whereas the LDA yields D_{3d} symmetry. Furthermore, the experimentally observed negative-U behavior of vacancy donor states is reproduced in the GGA results, but not in the LDA results. Both the LDA and GGA predict negative-U behavior for the vacancy acceptor states.

The formation energies of stable self-interstitial structures and the activation energies for transitions between these structures have been used as input to a Kinetic Monte-Carlo code, which is used to determine the diffusion rates as a function of temperature and carrier concentrations. For non-equilibrium carrier concentrations, fluctuations in the charge state of the self-interstitial lead to non-Arrhenius behavior via a modified Bourgoin-Corbett mechanism.

Significance—Developments in massively parallel software and computational techniques have enabled state-of-the-art calculations that provide key parameters critical to the future qualification of nuclear weapons components.

Sponsors for various phases of this work include: Nuclear Weapons/Qualification Alternatives to the Sandia Pulsed Reactor (QASPR) and Advanced Simulation & Computing (ASC)

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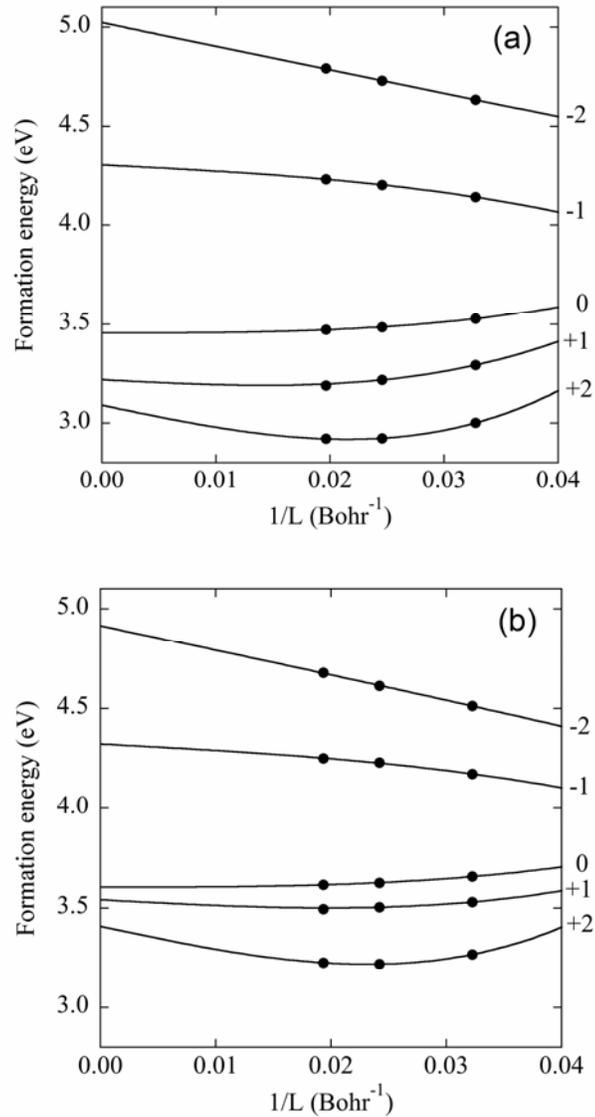


Figure 1. Plots of Si vacancy formation energies (in eV) versus $1/L$ (Bohr^{-1}) where L is the cubed root of the supercell volume. Filled circles indicate the formation energies computed in 215-, 511-, and 999-atom supercells. Lines show fits of the supercell data to Eqn. 1. The charge states, q , are given along the right side of the plot. a) Results obtained using the LDA. b) Results obtained using the GGA.