High Precision Quantum Mechanics Calculations for Silicon Defects

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Motivation—The QASPR (Qualification Alternatives to the Sandia Pulsed Reactor) program has the challenging task of developing a capability to accurately model gain degrada-tion and recovery in semiconductor devices following intense neutron irradiation, with the goal of using this capability to help qualify nuclear weapons. A foundational element of this modeling effort is density-functional-theory (DFT) calculations for the energy levels and migration enthalpies of the primary defects produced by the irradiation and the secondary defects produced by reactions of these defects with each other and with impurities or dopants. The importance of the QASPR program to the Laboratory motivated us to utilize Sandia's large-scale computers to overcome substantial obstacles that limited the precision of previous calculations for defects in semiconductors.

Accomplishment—We developed a method for eliminating the supercell size dependences that plagued all previous DFT calculations for defects in semiconductors and applied this method to obtain high precision results for the energy levels and migration enthalpies of the two primary defects in silicon: the Si vacancy and the self-interstitial. After describing the new method, we report a few of the results obtained for the Si vacancy.

Periodic boundary conditions are widely used in DFT calculations for defects in silicon. They yield an efficient computational scheme, but also introduce spurious electrostatic and strain interactions between the defect and its periodic replicas. These interactions can influence the defect atomic configuration and formation enthalpy, and ultimately cause the results to depend on the size of the supercell. This dependence is especially pronounced for charged defects, but is also present even for neutral defects. To eliminate this dependence, we computed defect formation enthalpies in supercells containing nominally 216, 512, and 1000 atoms, and fit these results to a physically reasonable formula to obtain the formation enthalpy in an infinite sized cell corresponding to an isolated defect. We did this not only for the local energy minimum configurations (LEMCs) (see Fig. 1), but also for the saddle point configurations (SPCs) which are traversed by a migrating defect. By subtracting the LEMC value from the SPC value, we obtained the migration enthalpy. Furthermore, we obtained the electronic energy levels in the band gap from differences in the LEMC formation en-thalpies.

The configurations found for the Si vacancy LEMCs were in agreement with results from experiments, and the energy levels near the bottom of the gap were within 20 meV of the experimental results (see Fig. 2 - experimental results are not available for the two levels higher in the gap). The Si vacancy migration enthalpies were within the range of measured values except for the -1 charge state, for which there is only one measured value. (There is no measured value for the +1 charge state.)

Significance—The rigor and precision of these DFT calculations are advancing understanding of defect physics and are providing confidence in the QASPR program and its ability to serve as an alternative methodology for qualifying nuclear weapons.

Sponsors for various phases of this work include: Nuclear Weapons/Advanced Simulation & Computing (ASC)/Physics and Engineering Models (PEM)

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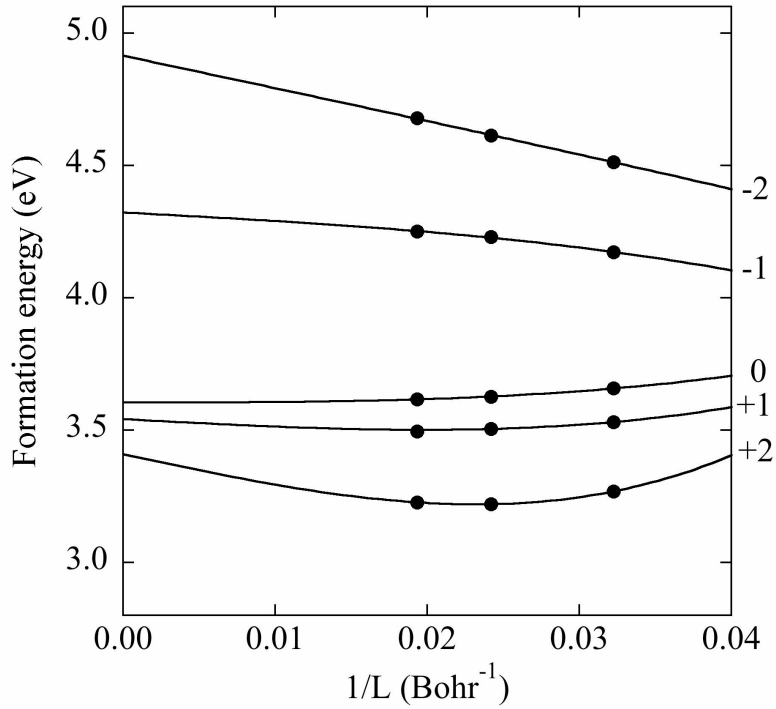

Figure 1. Plots of Si vacancy LEMC formation enthalpies versus the inverse of the length of the supercell. The filled circles are computed values, and the lines are fits.

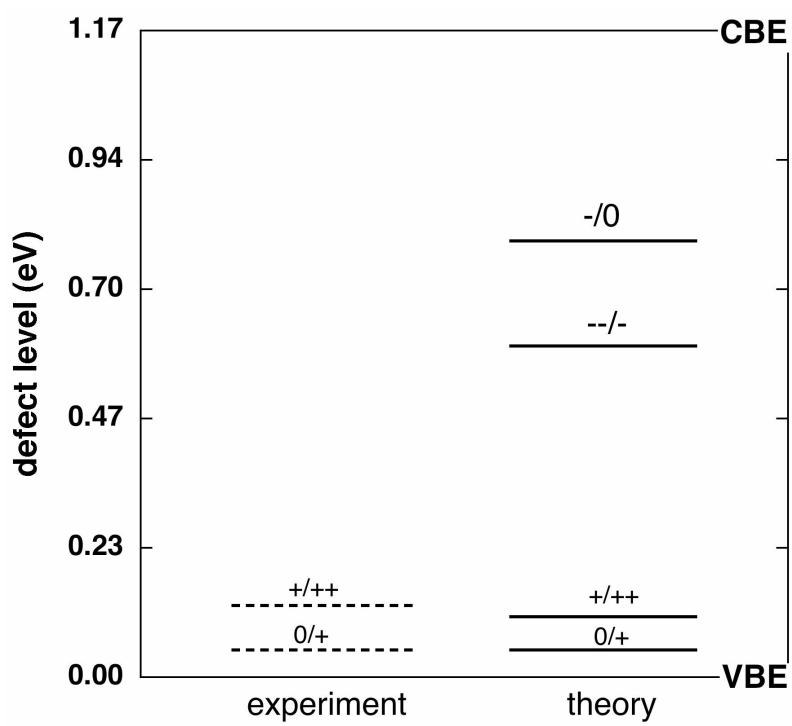

Figure 2. Experimental and theoretical Si vacancy energy levels.