

Modeling the Silicon Interstitial: Why the Self-interstitial is Invisible

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Motivation—One of the most enduring mysteries in the field of semiconductor defects is to explain why no one has observed the isolated self-interstitial defect in silicon. This defect, along with the silicon vacancy, is one of the primary defects created in silicon material and devices by high-energy electrons, ions, or neutrons. However, numerous experiments over the past 50 years have failed to directly observe the silicon self-interstitial.

Accomplishment—We have applied our state-of-the-art computational capabilities to model the silicon self-interstitial, and our results explain why it has escaped direct detection for so many years. In p-type silicon, various indirect experiments suggest that the interstitial escapes detection because it is highly mobile at temperatures as low as 4.2K in the presence of ionizing radiation. This was qualitatively rationalized many years ago by the so-called Bourgoin-Corbett mechanism of athermal defect migration. Figure 1 shows our calculated diffusion coefficient as a function of temperature in p-type material with varying rates of electron-hole recombination at the defect. Our calculations identify a specific mechanism of athermal diffusion that is a modification of the standard Bourgoin-Corbett mechanism. This process results in the temperature invariance of our calculated diffusion coefficient at low temperatures or high ionization levels.

In n-type silicon, we can explain why the self-interstitial defect has also escaped detection, in spite of indirect evidence that athermal motion is not taking place. It is known by observing the creation of carbon interstitials from mobile silicon interstitials via the well-known “kick-out” mechanism that silicon self-interstitials do

not move in n-type material until at least 150-175K. Thus one might expect the self-interstitial to be observable by Electron Paramagnetic Resonance (EPR) or Deep-Level Transient Spectroscopy (DLTS) experiments below this temperature. However, in spite of numerous attempts, this important defect has remained invisible. Figure 2 shows our stability results for various charge states and configurations of the self-interstitial as a function of Fermi energy. Two important and previously unrecognized properties of the silicon interstitial are predicted. First, the silicon self interstitial is “negative-U” or very nearly “negative-U” for both positive and negative charge states, i.e., only charge states with pairs of electrons or holes trapped at the defect are likely to occur in significant populations. The absence of unpaired spins explains the negative results of EPR experiments. Second, there is a wide region of stability of the 2^- charge state below the conduction band edge, and the defect moves at a temperature lower than the DLTS peak corresponding to thermal emission of trapped electrons. Thus the silicon self-interstitial is not observed in a DLTS spectrum, in agreement with numerous negative results. This is an interesting property of the defect, since it implies that—unlike most other defects—there is a lower thermal barrier for moving the defect than there is for emitting a trapped carrier.

Significance—All of these predicted properties that explain the “invisible” nature of the silicon interstitial are key metrics that give us confidence in the accuracy of our defect modeling capabilities that are critical inputs to the Qualification Alternatives to Sandia Pulse Reactor (QASPR) project.

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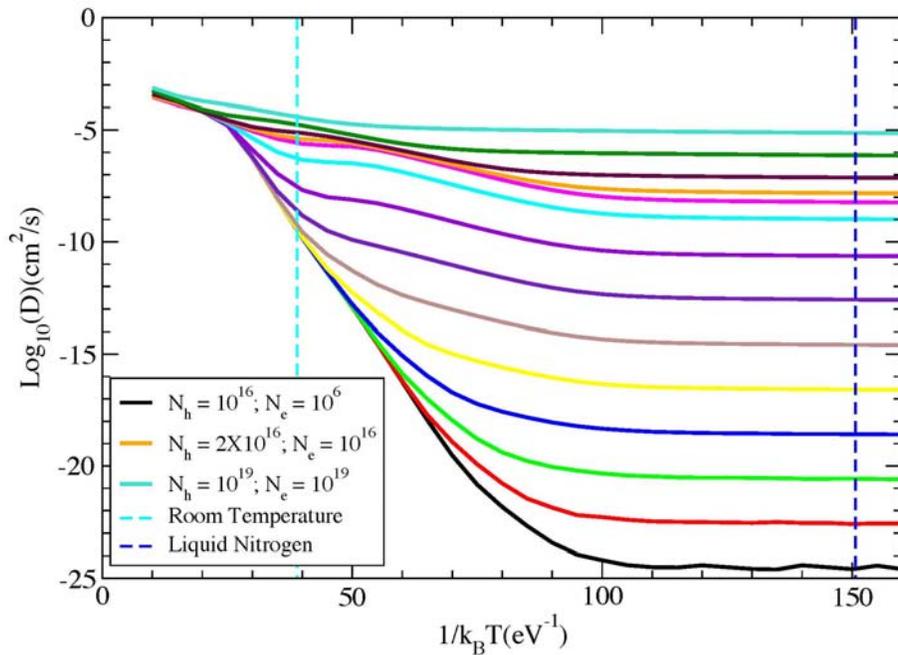


Figure 1. Diffusion coefficients as a function of inverse temperature obtained by incorporating diffusion barriers calculated using the Local Density Approximation (LDA) to the Kohn-Sham Density Functional Theory into a Kinetic Monte-Carlo simulation. Results are for a non-equilibrium p-type system with 10^{16} ionized acceptors and a variable number of additional electron-hole pairs.

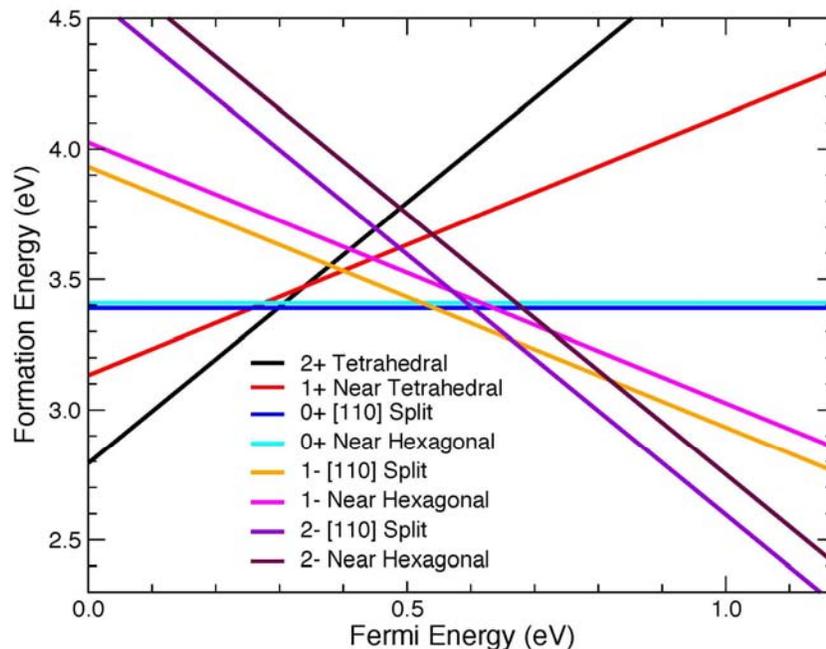


Figure 2. Thermodynamic stability diagram obtained from LDA calculations. The electronic Fermi energy is referenced to the valence band edge. The charge and configuration of the interstitial with the lowest formation energy is thermodynamically stable at a given Fermi energy.