Interstitial clusters in Si

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Interstitials are atoms that are positioned between or sharing normal lattice sites. Native interstitials that arise from the atoms that constitute the lattice itself are called self-interstitials. They are created inadvertently during ion implantation or by irradiating the sample with, say, protons with sufficient energy. These processes can lead to the formation of point and eventually extended defects depending on energy, dose and annealing temperature. These extended and planar defects are believed to induce transient enhanced diffusion of Boron, a limiting factor in controlling dopant profiles which hampers the further reduction in size of next-generation sub-micron semiconductor devices. Therefore it is highly desirable to develop a theory that describes the microscopic processes that occur during the formation of extended defects, namely the aggregation of small compact clusters to elongated chains and then "rod-like" defects oriented in the {311} plane. The latter defects range in size from 1-100 nm in width and up to 1 µm in length.

The growth of interstitial clusters can be studied theoretically by recently developed molecular dynamics schemes that allow one to record microscopic processes for time periods up to 1 µs with fs resolution. A super-cell of 512 Si atoms contains n additional Si interstitials and the atoms are subject to a classical many-body potential within the modified embedded atom method that is tested against *ab initio* calculations. The trajectory of all atoms and the total energy of each relaxed configuration are recorded allowing us to find stable or metastable structures. In particular, the method allows one to find candidates for the ground state structure of complex defect types such as the tri-interstitial I_3 or the tetra-interstitial I_4 consisting of an interstitial aggregate of three or four interstitials, respectively (Figs. 1 and 2).

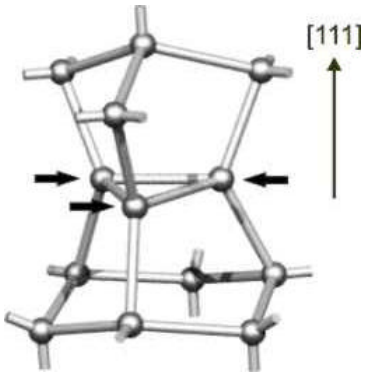

Fig. 1: *Tri-interstitial. The interstitials (arrows) are placed at three bond-centered sites. Remarkably, all atoms are four-fold coordinated. Although this defect is not the lowest energy structure for I_3, it could account for the W-line seen in photoluminescence experiments* [1].

It is important to augment these semiempirical studies by *ab initio* density functional calculations in order to reliably predict the energies and transitions paths of these structures. Several properties of point defects such as point group symmetries, deep levels in the band gap, optical transition energies, localized vibrational modes or localization of the wave functions can then be correlated to experimental data obtained from electron paramagnetic resonance (EPR), deep level transient spectroscopy (DLTS), photoluminescence (PL) or localized vibrational mode spectroscopy (LVMS) measurements.

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We now briefly discuss some of the highlights obtained by the molecular dynamics and *ab initio* calculations. Single interstitals I_1 are found to be very mobile and combine to di-interstitials I_2 or tri-interstitials I_3 that are also very mobile. Compact clusters containing up to 20 interstitials can be formed subsequently. However, compact clusters containing more than five atoms are found to be unstable with respect to the formation of elongated chains that are lower in energy. These elongated chains I_n act as traps for additionally introduced interstitials by capturing them eventually at the chain ends (Fig. 3) forming an I_{n+1} chain as the ground state structure.

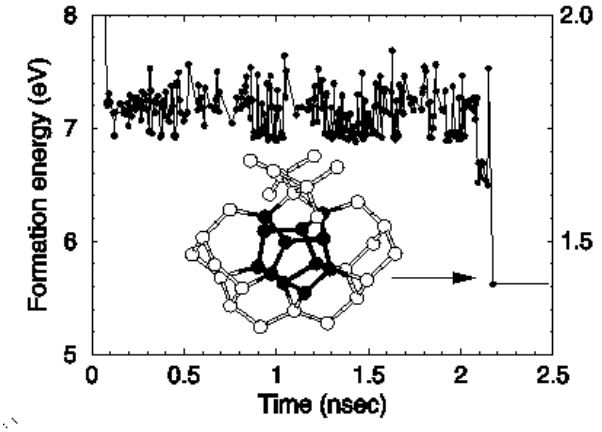

Fig. 2: *Formation energy of a tetra-interstitial during a parallel-replica run at 800 K and the core structure of the ground I_4-D_{2d} cluster. The starting configuration consists of four randomly distributed interstitials in a 512-atom cell. After 20 interstitial jumps, a metastable I_4 precursor is formed, releasing 5.4 eV (off the scale). Once the transition to I_4-D_{2d} occurs (arrow), no more transitions are observed within 10 nsec. Again, all atoms are four-fold coordinated.*

Our studies indicate that the energetically favorable shape of interstitial clusters evolves from compact to elongated and eventually "rod-like" {311} defects when more and more interstitials are being injected. Steady improvements of empirical potentials for silicon in combination with new algorithms reaching up to μsec time scales offer exciting opportunities to directly probe the critical steps of interstitial cluster growth.

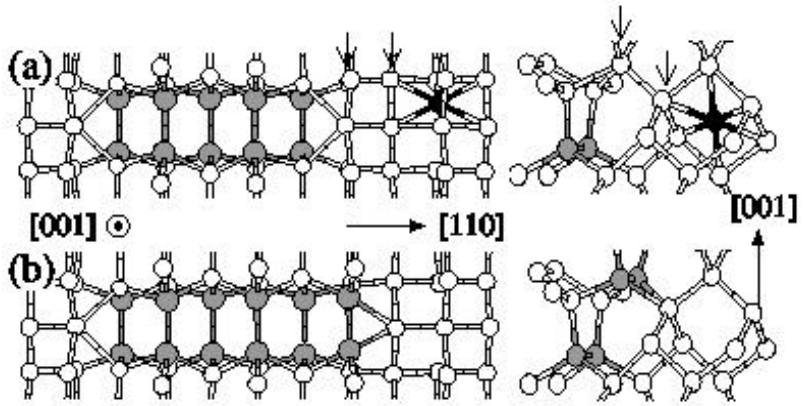

Fig. 3: *Schematics for an interstitial trap by an elongated chain.*
(a) An interstitial is placed at the nearest hexagonal site.
(b) An extra chain is formed by concerted motions of the interstitial and the atoms at the end, releasing 2 eV.

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