Contribution ID: **340** Type: **Oral Presentation**

Ab-initio study of the energy of formation and diffusion paths of self-interstitials in silicon

Thursday, 14 July 2011 14:00 (15 minutes)

<p>The formation energy of self-interstitial defects in silicon was studied. The 110split site was found to be the lowest energy position for the silicon self-interstitial at neutral charge state, as well as singly and doubly negative charged state. The tetrahedral site is found to be the lowest energy site for the singly and doubly charged positive states. The energy barriers for diffusion from the 110split site to the hexagonal and tetrahedral sites were found to be 0.370 and 0.361 eV respectively. Diffusion between the tetrahedral and hexagonal sites has an energy barrier of 0.074 eV. These energy barriers are found to be too great to account for athermal diffusion of the silicon self-interstitial, and diffusion paths involving cyclic changes in charge state are most likely to be responsible for the athermal diffusion observed at low temperature.

Level (Hons, MSc,
   PhD, other)?

Hons

Consider for a student
   award (Yes / No)?

Yes

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

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