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SEMINAIRE

Service de Recherches de Métallurgie Physique

DEN/DANS/DMN

Attention : horaire et lieu de réunion inhabituel :

SALLE du DRECAM/SPAM – Bâtiment 522 - Pièce 137 – 10h

Ab-initio stability and mobility of silicon single and di-interstitials in silicon carbide

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Via ab initio methods the structural stability and mobilities of single and di-silicon interstitials in their neutral state are investigated in 3C- and 4H-SiC. In 3C-SiC, the neutral silicon interstitial finds its global minimum energy configuration as the tetrahedrally carbon-coordinated interstitial closely followed by the split interstitial along <110> direction on silicon lattice site, which could be present in a significant amount as comparable to I_{TC} under high temperature growth and irradiation conditions. We also found that the convergence of formation energies vs Brillouin Zone sampling and supercell size is quite defect-type sensitive. For 4H-SiC, the most energetically favorable silicon interstitial is found to be the split interstitial configuration $I_{Sisp<110>}$ but situated in the hexagonal layer. I_{TC} and $I_{Sisp<110>}$ in 3C-SiC provide a mean to capture and integrate Si interstitial into a di-interstitial cluster, followed by a transition to the formation of di-interstitial ground state, which is identified as a split interstitial pair $I_{Sisp<001>}$ forming a triangular configuration on a <010> plane with one side along the <001> direction and a bisector along <100>. The nudged elastic band method reveals an easy reorientation character on the same lattice site, in-plan and out-of-plan, for this ground state structure. However, based on the analysis of the energy potential surface, we postulate that the silicon interstitial clusters would rather remain undisplaced once formed, and the long range diffusion be predominantly performed by single interstitial migration mechanism, in which case a frequent association and dissociation of silicon interstitial clusters should occur upon heating in SiC. The inferred compact-to-extended transition mechanism prevailing over the kick-out self-migration mechanism also suggests a role for the compact di-interstitial ground state in the nucleation of larger extended silicon network.

Vendredi 18 Janvier 2008 à 10h

N.B **:** ***Les visiteurs de nationalité étrangère hors Union Européenne sont priés de bien vouloir avertir impérativement 3 semaines à l'avance - les visiteurs de l'Union Européenne 1 ou 2 jours avant le séminaire - le Secrétariat du Service de leur entrée sur le Centre :***

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