Stability of neutral silicon interstitials in 3C- and 4H-SiC: A first-principles study

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The structural stability and properties of single silicon interstitials in their neutral state are investigated via \textit{ab initio} methods in 3C- and 4H-SiC. We find a strong dependence of defect formation energies on the choice of $k$-point sampling and confirm that $\Gamma$ point alone is far from sufficient to achieve the convergence if the supercell is not large enough. By using a larger $k$ grid ($2\times2\times2$ shifted-mesh) in 65-atom 3C-SiC, the neutral silicon interstitial find its global minimum energy configuration as split interstitial along $<110>$ direction on silicon lattice site, instead of the tetrahedrally carbon-coordinated interstitial configuration as reported by some previous works. For 4H-SiC, the most energetically favorable silicon interstitial is also found to be the split interstitial configuration $I_{\text{Sisp}}<110>$ but in the hexagonal layer. This result can be reasoned from the fact that an open structure of SiC along the $<110>$ direction allows for a relatively small relaxation around this interstitial and a larger energy gain compared to other cases. The defect formation energies in 4H-SiC are in general larger than those in 3C-SiC, implying that the insertion of silicon interstitial introduces a large lattice distortion to the local coordination environments and affect even the second- or thirdnearest neighbors. We present also some preliminary results on di-interstitials clusters. In the top of their hierarchy, two compact clusters are found, one is composed of a dumbbell along $<110>$ direction with a center silicon atom located nearby which resembles to a well-known structure in silicon, and the other consists of two split interstitials arranged in orthogonal directions, $I_{\text{Sisp}<001>}$ and $I_{\text{Sisp}<110>}$.

Number of words in abstract: 260

Keywords:
Technical area: 11. Multiscale modeling for fusion materials and structure
Special session: Not specified
Presentation: No preference
Special equipment: No special equipment