From point defects to the extended structure in Si

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Molecular dynamics combined with the nudged elastic band method reveals the microscopic self-diffusion process of compact silicon tri-interstitials. During the diffusion, a five defect-atom entity both translates and rotates in a screw-like motion along $\langle 111 \rangle$ directions with a diffusion barrier of 0.5 eV. The low-diffusion barrier suggests that the compact tri-interstitial is highly mobile and may play an important role in the growth of ion-implantation-induced extended interstitial defects.

The combination of tight-binding molecular dynamics and density functional theory reveals a possible growth mechanism of silicon interstitial chains from the compact silicon tri-interstitial[1]. We estimate the transition rate from a compact tri-interstitial to ground state tri-interstitial is 7.8 THz $\exp(-1.4/k_BT)$. The ground state tri-interstitial cannot directly develop into a short interstitial I_3-chain, which can readily decay to a ground state tri-interstitial with a barrier of ~ 100 meV. On the other hand, the ground state tri-interstitial can develop into a I_4-chain with a strong exothermic reaction by capture of a single interstitial, which starts the growth process of a interstitial chain.

[1] D. A. Richie *et al.*, Phys. Rev. Lett. **94**, 0445501 (2004).