Fast Diffusion Mechanism of Silicon Tri-interstitial Defects

Yaojun Du, Kaden R. A. Hazzard, R. G. Hennig, and J. W. Wilkins

Department of Physics, The Ohio State University
Columbus, OH, USA

We reveal the microscopic self-diffusion process of compact tri-interstitials using a combination of molecular dynamics and the nudged elastic band method. Five atoms diffuse collectively in a screw-like motion in the [111] directions. This self-diffusion can be described by the translation and rotation of these five atoms. The discovery of this pathway demonstrates the utility of combining tight-binding molecular dynamics with *ab initio* energetics calculations to probe diffusion mechanisms. The pathway estimates a diffusion constant of $0.2\ 10^{-5}\ \exp(-0.48\ \mathrm{eV}/k_BT)\ \mathrm{cm}^2/\mathrm{s}$, compared to $\sim 10^{-5}\ \exp(-0.4\ \mathrm{eV}/k_BT)\ \mathrm{cm}^2/\mathrm{s}$, the experimental diffusion constant for Si interstitials. This suggests that the self-diffusion of compact tri-interstitials is a dominant mechanism for the diffusion of Si interstitials.

We also show that the compact tri-interstitial can transform to an extended structure[1]. This extended structure can capture a single interstitial to develop a four-interstitial chain.

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