

Abstract Submitted
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Pathway connecting the four-interstitial ground state and chain in silicon YAOJUN DU, Wake Forest University, THOMAS LENOSKY, 879 Meadowview Dr, Columbus OH 43224, STEFAN GOEDECKER, University of Basel, RICHARD HENNIG, JOHN WILKINS, The Ohio State University — Dimer searches, minima hopping and nudged elastic band (NEB) calculations try to identify the lowest pathway connecting the two important silicon four-interstitial structures: I_4 -chain and ground state. First, 400 tight-binding dimer searches reveal several local minima. However, the minima have high DFT formation energies and no pathway connecting chain and ground state is found. Second, we fit a classical modified embedded atom method potential to a database of interstitial clusters. Minima hopping using this potential finds several structures with DFT energies between chain and ground state but no pathway connecting them. Finally, we construct a pathway between chain and ground state with small displacements. The NEB energy barrier with DFT from chain to ground state is 0.6 eV. This indicates that during annealings the I_4 -chain decays into the nearly immobile ground state, implying that chain structures predominate only for longer chains.

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