Abstract

Kinetic effects have proven to play a decisive role in many structural transitions in Si and Ge. Despite both elements being prototype and industrially widely used semiconductors, these phenomena are not well understood. We have studied kinetic effects using enhanced sampling methods, mainly metadynamics, to comprehensively map transition pathways and barriers separating structural phases in Si and Ge. Because of high computational cost and need of good transferability we employed and tested multiple neural network potentials complemented by DFT methods to work in tandem with metadynamics. With these tools we have tried to systematically study structural phase transitions in Si and Ge in region of pressures lower than 10 GPa. We have identified multiple limitations of the proposed approach mainly in training a universally accurate trained potential along with possible solutions to these problems. Our goal is to improve the current understanding of phase transitions including kinetics and reach a better agreement between simulations and experiment, beyond the level of thermodynamic predictions.