From diamond to BC8 to simple cubic and back: Kinetic pathways to post-diamond carbon phases from metadynamics

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Abstract

Understanding the kinetic pathways connecting carbon polymorphs at multimegabar pressures remains a major unsolved problem in high-pressure physics. Here, we provide insights into the long-standing question of BC8 formation and stability by combining a state-of-the-art SNAP machine-learning interatomic potential with enhanced sampling via metadynamics, enabling direct access to transition mechanisms far beyond the reach of standard molecular dynamics. Our simulations show that carbon phase transformations are intrinsically complex, proceeding through multiple intermediate disordered and crystalline states governed by nontrivial kinetic ordering. We determine the upper pressure limit for BC8 formation and reveal that hexagonal diamond transforms to BC8 faster than cubic diamond—an unexpected and experimentally testable prediction. We also identify a *P*222 carbon phase that becomes competitive with diamond and simple cubic above 1.8 TPa, and we demonstrate that BC8 may be quenched to ambient conditions at moderate temperatures. Together, these results establish a general and transferable framework for resolving kinetic pathways in solid-solid phase transitions and provide physical insights into carbon's complex high-pressure landscape.

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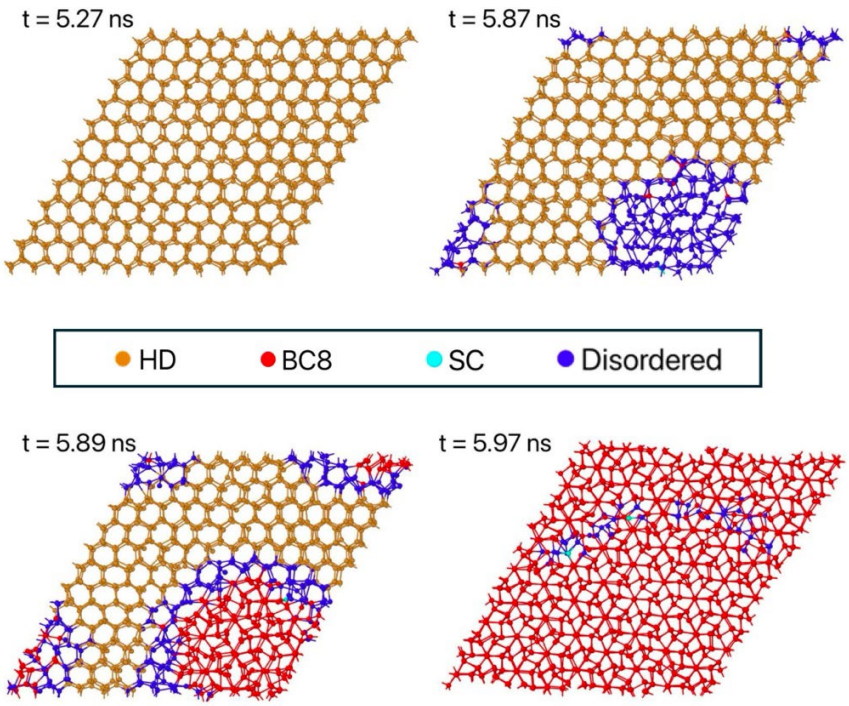

Transition from hexagonal diamond to BC8.