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Predictive simulations of metastable phases of carbon at high compression ASHLEY WILLIAMS, KIEN NGUYEN CONG, JONATHAN WILLMAN, University of South Florida, NIR GOLDMAN, Lawrence Livermore National Laboratory, IVAN OLEYNIK, University of South Florida — Carbon exhibits a relatively simple phase diagram under hydrostatic compression: thermodynamically stable sp2-bonded graphite and metastable sp3-bonded cubic diamond at ambient conditions and bc8 and simple cubic phases at high pressures above 1 TPa. There have been reports of appearance of hexagonal phase of diamond in shock experiments, but these results have been questioned by interpreting associated diffraction peaks as deformation twinning on (111) planes as a result of plastic deformations in cubic diamond. We explore unknown metastable phases of carbon under both hydrostatic and uniaxial compression by using combination of first-principles density functional theory and semi-empirical density functional tight-binding combined with evolutionary crystal structure prediction. Shear stresses play a key role in transformation of diamond to new lower energy metastable phases. Their appearance provides a plausible interpretation of recent experimental observations.

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