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Synthesizability of Superhard Carbon by Cold Compression of Graphite[1] SALAH EDDINE BOULFELFEL, ARTEM OGANOV, Stony Brook University SUNYSB, STEFANO LEONI, Technical University Dresden — We present an efficient scheme combining Monte Carlo walk in the space of transition pathways with molecular dynamics simulations for predicting matter modification under high pressure. If crystal structure prediction is a top-interest field for science and technology, the quest is even more exciting for elements such as boron and carbon. While under pressure above 15 GPa and at high temperatures (1600-2500 K) graphite is converted into diamond, room temperature compression gives a new superhard modification of carbon. Its nature remained unresolved until recent theoretical investigations predicted two candidate structures, M-Carbon and BCT4. Both structures have comparable physical properties and refine well the XRD data. To elucidate the nature of the final product of graphite cold compression we performed molecular dynamics transition path sampling simulations and we determined the energy profile of each transition (graphite to M-carbon and graphite to BCT4). The intrinsic mechanism of the reconstruction and the reasons of the favoring of one structure over the other have been determined. A detailed picture of events of nucleation and growth during the transition is finely reproduced. Our procedure do not only determine the nature of a transition final product but predicts its synthesizability under given conditions of pressure and temperature.

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