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Prediction of a new metastable sp^3-carbon allotrope at ambient conditions TAKASHI MIYAKE, Research Institute for Computational Sciences, AIST, Japan, KOICHIRO UMEMOTO, Geology and Geophysics, University of Minnesota, RENATA WENTZCOVITCH, Chemical Engineering and Matarials Science, University of Minnesota, SUSUMU SAITO, Physics, Tokyo Institute of Technology, Tokyo, Japan — We have investigated by first principles the viability of a new form of sp^3 crystalline carbon recently found in tight-binding molecular dynamics simulations of carbon nanotubes (CNT) under pressure. It consists of unique 4-membered rings and has body centered tetragonal structure (henceforth bct-C_4). It is also a polymerized form of (2,2) CNT, the smallest CNT. This phase is dynamically stable at zero pressure and is more stable than graphite beyond 18.6 GPa. At zero pressure it is also more stable than fcc C_{60} and (7,0) and (8,0) CNTs. Inspection of this transparent polymorph shows a peculiar relationship with hexagonal diamond, which suggests that this phase might be an intermediate phase along the graphite to hexagonal diamond transformation path. This possibility appears to be supported by the good match between the simulated x-ray diffraction pattern of bct-C_4 and that of an intermediate transparent and hard phase of carbon produced by cold compression of graphite.

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