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Transforming graphite to diamond: An *ab initio* molecular dynamics study of graphite under shock compression[1] CHRISTOPHER J. MUNDY, Pacific Northwest National Laboratory, NIR GOLDMAN, I-F. WILLIAM KUO, EVAN J. REED, LAURENCE E. FRIED, Lawrence Livermore National Laboratory, ALESSANDRO CURIONI, IBM Research - Zurich — We present an extremely large scale *ab initio* calculation of the transformation of graphite to diamond under shock compression utilizing Car-Parrinello Molecular Dynamics (CPMD) in conjunction with the Multi-Scale Shock Method (MSSM). Our results indicate that the transition from graphite to diamond is Martensitic, in agreement with experimental observations. We find that a shock of 12 km/s forms a short-lived layered diamond phase which eventually relaxes to a cubic diamond state. Moreover, access to the electronic structure allows the computation the x-ray absorption spectra (XAS) to characterize the final states. The XAS spectra and wide angle x-ray scattering spectra (WAXS) confirm the presence of a cubic diamond final state.

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