First-Principles Calculation of the Diamond Shock Hugoniot

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The phase diagram of carbon at high pressures and temperatures is of scientific interest to material science, geology and astrophysics. The advent of the diamond anvil cell has made the study of materials at extreme hydrostatic pressures possible. Carbon's diamond phase is the hardest and least compressible material occurring in nature. As a result, the properties of diamond at extreme pressures remain mostly unknown. Recently [1], diamond was compressed to a conducting fluid by laser generated shock. Reflectance data showed that diamond undergoes a continuous transition from optically absorbing to reflecting at Hugoniot pressures 600 - 1000 GPa. We report preliminary results for the shock Hugoniot of diamond calculated using the DFT-PAW formalism as implemented in the VASP code [2].

[1] D. K. Bradely, J. H. Eggert, D. G. Hicks and P. M. Celliers, S. J. Moon, R. C. Cauble, and G.W. Collins, Phys. Rev. Lett. **93**, 195506-1 (2004).

[2] http://cms.mpi.univie.ac.at/vasp