Abstract Submitted
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Density Functional Theory simulations of shock compression of porous tantalum pentoxide[1] K. COCHRANE, T.J. VOGLER, S. ROOT, M.P. DESJARLAIS, L. SHULENBURGER, T.R. MATTSSON, Sandia National Laboratories — Density Functional Theory (DFT) based molecular dynamics has been established as a method capable of yielding high fidelity results for many materials at a wide range of pressures and temperatures and has recently been applied to complex polymers such as polyethylene, compounds such as ethane or CO_2, and oxides such as MgO. We use this method and a modification to the Rankine-Hugoniot relation inspired by the P-_crush model to extend the DFT approach to the calculation of the shock response of an initially porous tantalum pentoxide. The experimental data have initial densities of approximately 1 g/cc, 3 g/cc, and 7 g/cc, reduced from a normal density of 8.36 g/cc, with final pressures up to 200 GPa. The DFT results compare well with the 3 g/cc and 7 g/cc over a wide range of pressures. The agreement with the 1 g/cc Hugoniot experimental data is reasonable at lower pressures, but with some larger discrepancies at higher pressures. Finally, we calculate the Gruneisen gamma as a function of density and found that it is density dependent but pressure independent for the lower densities and higher pressures. These results show that DFT methods may be capable of dealing with highly distended material with the proper modifications.

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