Abstract Submitted
for the DPP15 Meeting of
The American Physical Society

Quantum molecular dynamics simulations of argon along the multi-shock Hugoniot line HUAYANG SUN, DONGDONG KANG, JIAYU DAI, JIAOLONG ZENG, JIANMIN YUAN, National University of Defense Technology
— The equation of states of argon along the multi-shock Hugoniot line from 0.02 eV, 0.5 g/cc to 3 eV 5.5 g/cc are calculated by the pair potential and the first principles calculations with and without van der Waals corrections. The calculations of 273 K isothermal line from 0.5 to 5.5 g/cc show that: (a). at 0.5 g/cc, the precision increase from Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional without vdW correction, PBE exchange-correlation functional with force-field corrections method by Grimme (DFT-D), van der Waals density functional method of version 2 (vdW-DF2), to pair potential [1]; (b). the pair potential and vdW-DF2 tend to overestimate the pressure at high densities. The pressures above 1 eV show that DFT-D gives consistent results with PBE, which are larger than those of the pair potential, while the pressures of vdW-DF2 increase a little quickly with temperature. The Hugoniot lines of DFT-D are consistent with the 1st shock results of the experiments [2], but have departures with the results after the 1st shock.

[1] K. Patkowski et al., Molecular Physics 103:15-16, 2031 (2005).
[2] Q. F. Chen et al., J. Chem. Phys. 140, 074202 (2014)
[3] Jiayu Dai et al. Phys. Rev. Lett. 109: 175701 (2012).

Zengxiu Zhao
National University of Defense Technology

Date submitted: 24 Jul 2015 Electronic form version 1.4