Commun. Comput. Phys.
doi: 10.4208/cicp.290411.121211a

Vol. **12**, No. 4, pp. 1121-1128
October 2012

First-Principles Calculations of Shocked Fluid Helium in Partially Ionized Region

Cong Wang[1], Xian-Tu He[1,2] and Ping Zhang[1,2,*]

[1] *LCP, Institute of Applied Physics and Computational Mathematics, P.O. Box 8009, Beijing 100088, China.*

[2] *Center for Applied Physics and Technology, Peking University, Beijing 100871, China.*

Received 29 April 2011; Accepted (in revised version) 12 December 2011

Communicated by Xingao Gong

Available online 17 April 2012

Abstract. Quantum molecular dynamic simulations have been employed to study the equation of state (EOS) of fluid helium under shock compressions. The principal Hugoniot is determined from EOS, where corrections from atomic ionization are added onto the calculated data. Our simulation results indicate that principal Hugoniot shows good agreement with gas gun and laser driven experiments, and maximum compression ratio of 5.16 is reached at 106 GPa.

AMS subject classifications: 81Q05, 82D10, 85A04

Key words: Equation of state, warm dense matter, ab initio simulations.

1 Introduction

High-pressure introduced response of materials, which requires accurate understandings of the thermophysical properties into new and complex region, has gained much scientific interest recently [1]. The relative high temperature and high density are usually referred as the so-called ”warm dense matter” (WDM)—a strongly correlated state, where simultaneous dissociations, ionizations, and degenerations make modelling of the dynamical, electrical, and optical properties of WDM extremely challenging [2]. WMD, which provides an active research platform by combining the traditional plasma physics

---

[*] Corresponding author. *Email addresses:* `wang_cong@iapcm.ac.cn` (C. Wang), `xthe@iapcm.ac.cn` (X.-T. He), `zhang_ping@iapcm.ac.cn` (P. Zhang)

and condensed matter physics, usually appears in shock or laser heated targets [3], inertial confinement fusion [4], and giant planetary interiors [5].

Next to hydrogen, helium is the most abundant element in the universe, and physical properties of warm dense helium, especially the EOS, are critical for astrophysics [6,7]. For instance, the structure and evolution of stars, White Dwarfs, and Giant Planets [8–11], and therefore the understanding of their formation, depends sensitively on the EOS of hydrogen and helium at several megabar regime. For all planetary models, accurate EOS data are essential in solving the hydrostatic equation. As a consequence, a series of experimental measurements and theoretical approaches have been applied to investigate the EOS of helium. Liquid helium was firstly single shocked to 15.6 GPa using two stage light gas gun by Nellis *et al.*, then double shocked to 56 GPa, and the calculated temperature are 12000 and 22000 K respectively [12]. Maximum compression ratio (η_{max}≈6) was achieved by laser driven shock experiments with the crossover pressure around 100 GPa [13], However, soon after that, Knudson *et al.* have modified η_{max} to be 5.1 [14]. Theoretically, since the ionization equilibrium is not interfered with the dissociation equilibrium between molecules and atoms, helium, which is characterized by monoatomic molecule and close shell electronic structure, is particularly suitable for the investigation of the high pressure behavior under extreme conditions. Free energy based chemical models by Ross *et al.* [15], Chen *et al.* [16], and Kowalski *et al.* [17] have been used to investigate the principal Hugoniot of liquid helium, and the results are accordant with gas gun experiments. However, considerable controversies have been raised at megabar pressure regime, especially since the data was probed by laser shock wave experiments. Interatomic potential method predict η_{max}=4 for shock compressed helium [15], whereas, the EOS used by the astrophysical community from Saumon *et al.* (SCVH) [8], path-integral Monte Carlo (PIMC) [18], and activity expansion (ACTEX) [19] calculations provide an increase in compressibility at the beginning of ionization. For the initial density of ρ_0=0.1233 g/cm^3, SCVH and ACTEX simulation results indicate the maximum compression ratio lies around 6 at 300 GPa and 100 GPa respectively [8,19], while PIMC calculations suggest η_{max}=5.3 near 360 GPa [18].

On the other hand, quantum molecular dynamic (QMD) simulations, where quantum effects are considered by the combinations of classical molecular dynamics for the ions and density functional theory (DFT) for electrons, have already been proved to be successful in describing thermophysical properties of materials at complex conditions [20,21]. However, the DFT based molecular dynamic simulations (with or without accounting for excited electrons) do not provide reasonable results at the ionization region, mainly because the atomic ionization is not well defined in the framework of DFT. Considering these facts mentioned above, thus, in the present work, we applied the corrected QMD simulations to study shock compressed helium, and the EOS, which is compared with experimental measurements and different theoretical models, are determined for a wide range of densities and temperatures. The calculated compression ratio is substantially increased according to the ionization of atoms in the warm dense fluid.