AB INITIO SIMULATION OF WARM DENSE ARGON

Sartan R.A.

JIHT RAS, Moscow, Russia
r.sartan@gmail.com

Warm dense argon is studied within the framework of the molecular dynamics method whit the use of density functional theory. A total of 8 isotherms are calculated in the temperature range of $T = 4000 - 25000$ K and density range of $\rho = 1 - 20$ g/cm^3. The pressure increases smoothly with the increase of density along the isotherms without any density discontinuities.

The electrical conductivity is calculated along the isotherms. A qualitative similarity with the results of analytical models is obtained [1, 2]. The isotherms have minima, which are smoothed out with the increase of temperature, although the positions of the minima differ by orders of magnitude in both by conductivity and by density. In any model, the isotherms converge at high density, which can be interpreted as a transition to a metal-like state. The conductivity of warm dense argon changes smoothly both with an increase in density and with an increase in temperature. The latter indicates the absence of a plasma phase transition, since it implies a discontinuity in conductivity.

The molecular dynamics results quantitatively differ from the experimental data [3]. The shock adiabat [3] is obtained in the range of densities $\rho = 2.5 - 3.5$ g/cm^3 and temperatures $T = 7300 - 24400$ K. The experimental temperature is about 2 times higher than the predicted one in this work and analytical models [1, 2]

Additionally, the concentration of free electrons and the plasma nonideality parameter Γ are estimated. The nonideality parameter varies from 5 to 50 depending on temperature and density. The dependence of Γ on the density ρ along the isotherms is close to $\Gamma \sim \rho^{0.33}$.

This work is supported by the RFBR grant 19-08-01135.

---

1. Fortov V. E., Ternovoi V. Ya., Zhernokletov M. V., Mochalov M. A., Mikhailov A. L.,Filimonov A. S., Pyalling A. A., Mintsev V. B., Gryaznov V. K. and Iosilevskii I. L. // J. Exp. Theor. Phys. 2003. V. 97., P. 259.
2. Homkin A. L., Shumihin A. S. // J. Exp. Theor. Phys. 2019. V. 59., P. 859.
3. Gatilov L. A., Gluhodedov V. D., Grigor'ev F. V., Kormer S. B., Kuleshova L. V. and Mochalov M. A. // PMTF. 1985. V. 1., P. 99.