Simulation of thermodynamic and transport properties of strongly coupled plasma by quantum molecular dynamics

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In this work we present first-principle simulation of thermodynamic, transport and optical properties of strongly coupled plasma at densities near the normal for a given substance and temperatures less than 10 eV. The quantum molecular dynamics method implemented in the VASP code [1] is applied. For comparison with available experimental thermodynamic data all types of shock-wave data is used: shock compression of solid and porous samples, adiabatic expansion, quasi-isentropic compression and sound velocity measurements behind the shock front. The simulated substances are metals (aluminum, copper, silver, gold) and deuterium. We investigate both thermodynamic and transport properties (complex dielectric function, thermal conductivity) and compare the results with available models. In most cases we obtain very good agreement with experimental data. Discrepancies from traditional theoretical models is discussed, in particular, the violation of the Wiedemann-Franz law. We use the calculated data for calibration of semiempirical models of equation of state and transport properties. In the last case we get the expression which consists of the sum of Lorentz poles and can be used for direct simulation of radiation absorption in metals and dielectrics.

References

1. Kresse G., Hafner J. Ab initio molecular dynamics for liquid metals. Phys. Rev. B. 1993. V. 47. P. 558-561.