First-principle computational methods FOR thermodynamic and transport properties of non-ideal metallic plasma

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Non-ideal plasmas appear in many problems of modern physics, including in existing and perspective power plants, at the interaction of powerful fluxes of electromagnetic radiation with matter, in high-current devices, in astrophysics, geophysics, metallurgy, etc. In particular, liquid metals and electrolytes should be considered as plasmas with strong interparticle interaction to describe their physical properties. Besides, dense metallic plasma contains a strongly degenerate electronic subsystem that dramatically hinders an adequate theoretical analysis. It is not surprising that up to now only quite rough qualitative models for the calculation of thermodynamic and transport properties of non-ideal plasma existed. The appearance of classical atomistic methods of simulation such as Monte Carlo and molecular dynamics substantially improved the description of classical plasma models such as the one-component plasma [1] and completely ionized two-component plasma [2]. Nevertheless, for degenerate systems the classical approaches are invalid even at the qualitative level.

In the presentation the review of the so-called first-principle computational methods of thermodynamic, transport and optical properties of strongly non-ideal degenerate plasma will be given. First-principle in this case means that no empirical information is used except for the charge and mass of nuclei and fundamental physical constants. The following approaches will be considered: semiclassical Thomas-Fermi model with various corrections, average atom models [3], path integral Monte Carlo methods [4], density functional theory and quantum molecular dynamics [5]. Simulation results will be compared with shock-wave experimental data and with experiments for liquid metals; additionally, some first-principle estimations of critical parameters of metals will be given. For transport and optical properties, the following methods will be applied: kinetic models with the relaxation time approximation, Ziman model, Kubo-Greenwood formula and Kramers-Kronig transformation. The results will be compared with experimental data on static and dynamic experiments. The analysis of different methods shows that modern approaches based upon quantum molecular dynamics and Kubo-Greenwood formula allows one to calculate all thermophysical properties of non-ideal plasma with good accuracy using one and the same theoretical model. This fact, in turn, opens the possibility to create wide-range approximation models of the new generation which are necessary for the continuum simulation of interaction of intense power fluxes with metals. The work is supported by RSCF, grant 20-42-04421.

References

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