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Study of transport properties of warm dense matter on the basis density functional theory

M.K. Issanova[1,2], S.K. Kodanova[1,2], T.S. Ramazanov[1,2], N. Djienbekov[1,2]
[1] Al-Farabi Kazakh National University, Almaty, Kazakhstan,
[2] Institute of Applied Sciences and Information Technology, Almaty, Kazakhstan,
e-mail (speaker): issanova@physics.kz

Warm dense matter is intensively studied all over the world both experimentally and theoretically. At high temperatures and pressures, the existing theoretical models of liquid, gas, solid and plasma are inapplicable to the extreme state of matter. The main obstacle to the application of these models is the strong non-ideality of the medium, that is, the significant role played by the interaction of particles and quantum effects.

Warm dense matter is formed during electrical explosion of conductors [1], on accelerator walls under the influence of strong electromagnetic fields, in solids and metal clusters under the influence of laser pulses or powerful particle beams [3–5] in shock-wave experiments [6–9], etc. The transport parameters of non-ideal plasma are also necessary for constructing models of inertial thermonuclear fusion, the behavior of astrophysical objects (white dwarfs, the internal structure of giant planets), and diagnostics of matter using X-ray Thomson scattering [10]. Beryllium is one of the most well-studied materials under normal conditions, and is also intensively studied under conditions of extreme pressure and temperature. The case of beryllium under extreme conditions is of primary interest for understanding the processes in planetary cores, both in the liquid state and in the solid state at high temperature and pressure [11].

Due to the difficulties of diagnostics under extreme conditions in experiments, quantum molecular dynamics (QMD) simulation based on the density functional theory has become an integral part of modern studies of heated dense matter. In this work, we present the results of calculations of the transport properties of beryllium using methods based on density functional theory (DFT simulation). Today, the density functional theory (DFT) is the most powerful tool for modeling the electronic structure and related physical properties of heated dense matter. Using DFT calculations, the electron density distribution of a quantum system in an equilibrium state (with the lowest free energy) is found. Then, such physical properties of warm dense matter as the density of electron states, bulk modulus, permittivity, electrical conductivity, and many others can be determined. We have computed transport coefficients on the basis of DFT-simulation for various values of parameters of warm dense beryllium.

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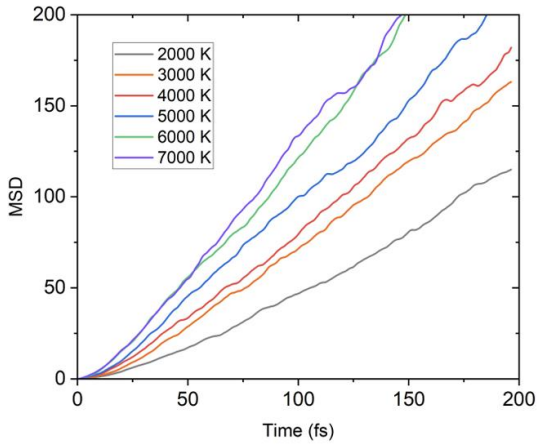

Figure 1. Mean Squared Displacement by DFT simulation

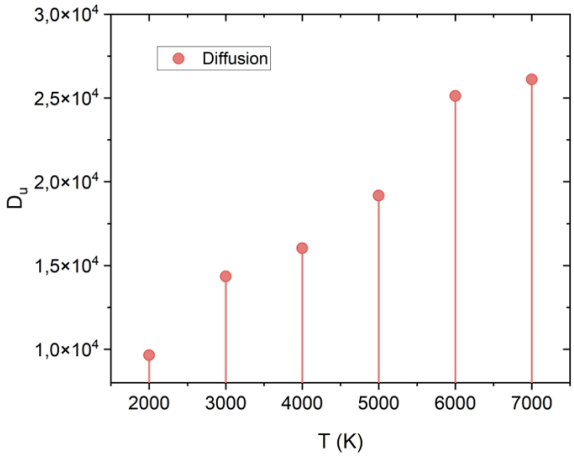

Figure 2. Diffusion coefficients using Einstein's relation by DFT simulation