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Ab-initio calculation of electrical and thermal conductivity of warm dense matter

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Warm dense matter (WDM) can be attributed to the state of matter at near-solid densities and temperature between 1 eV and 100 eV. Such conditions are believed to exist in the core of giant planets such as Jupiter and Saturn. Investigation of WDM is important for number of technological applications such as surface treatment at nanoscale (see for example [1]), laser deposition, creating plasma sources of X-rays and development of Inertial Confinement Fusion.

In this work, we present a direct calculation of thermal conductivity based on density functional theory and the Kubo-Greenwood formula [2, 3, 4, 5]. This method proved to be useful for modeling the transport properties in a wide range of densities and temperatures [5]. Two cases are considered: equilibrium, where temperature of electrons (T_e) equals temperature of ions (T_i) and nonequilibrium T_e » T_i. Electrical and thermal conductivity of aluminum and gold, typical s- and d- metals, is examine The calculations are performed for both liquid and solid phases in the range of Te from 0 to 6 eV.

Calculation of transport properties requires accurate determination of the electronic structure. This imposes a limit on the number of atoms considered so advanced calculations are conducted for 2000 atoms [6]. To perform typical calculations require the use of 1000 cores on a supercomputer, and 100 GB of memory per node.

[1] Norman G., Starikov S., Stegailov V., et al. *Nanomodication of gold surface by picosecond soft x-ray laser pulse* // J. App. Phys. 2012. V. 112. P. 013104.
[2] Zhilyaev P. and Stegailov V. *Ab initio molecular dynamics: application perspectives of multi-CPU and hybrid supercomputers* // Num. Meth. And Prog. 2012. V. 13. P. 37.
[3] Norman G., Starikov S., Stegailov V. et al. *Atomistic Modeling of Warm Dense Matter in the Two-Temperature State* // Contrib. to Plasma Phys. 2013. V. 53. P. 129
[4] Norman G., Saitov I., Stegailov V.. Zhilyaev P. *Atomistic modeling and simulation of warm dense matter. Conductivity and reflectivity* // Contrib. to Plasma Phys. 2013. V. 53. P. 300
[5] Norman G., Stegailov V., Zhilyaev P. Ab-initio calculation of thermal conductivity for metals with hot electrons // Doklady Akademii Nauk (in press)
[6] Pozzo M., Desjarlais M.P., Alfe D. *Electrical and thermal conductivity of liquid sodium from _rst-principles calculations* // PRB 2011. V. 84. P.054203.