Equation of State and opacities for warm dense matter

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This work presents a study of thermodynamic and trasport properties for matter at moderate and high temperatures and densities, including warm dense matter (WDM). This data is used in the AMR radiation transport code ARWEN [1] to study laboratory astrophysics and other processes like fast ignition (related to the HiPER project) or X-ray secondary sources (related to ELI project).

A general equation of state (EOS) obtained with QEOS is corrected with a new pressure multiplier (with density and temperature dependance) to fit the avaliable shockwave experimental data. Ab initio molecular dynamic (MD) simulations were done to improve the fitting for states where there is few avaliable data, as for WDM. The MD simulations uses the isokinetick esemble, keeping temperature and density fixed during the simulation. The equation of motion of the ions in contact with a thermostat are solved using the ABINIT code [2] in the framework of finite temperature density functional theory (DFT). The maximum temperature used in MD simulations are limited to 500 eV because of the calculations becomes prohibitive. An accurate EOS is obtained for a wide interval of densites and temperatures. All corrections in the EOS paid specially attention to his thermodynamic consistency to ensure the stability of the hydrodynamic code ARWEN.

Also ARWEN code includes heat transport process. The thermal conductivity coefficient is obtained using DFT with local density approximation (LDA), averaging over several time steps of a MD simulation. A detailed electronic structure calculation of the system is needed in order to obtain accurate results. Thermal conductivity is evaluated with the Kubo-Greenwood formulation. Great difference between analytical models [3] and DFT data exists for low temperatures where the ion correlation is important.

Finally, direct computation of the opacity of a mixture is compared with calculations that use an average over the opacities of pure elements. Also a comparison of the ionization derived from opacity calculations with the predicted ionization of the Thomas-Fermi model is done because of his importance in radiation process.

References:

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