PRESSURE IN ELECTRONICALLY EXCITED WARM DENSE METALS

V. V. Stegailov, P. A. Zhilyaev

*Joint Institute for High Temperatures RAS, Izhorskaya street, 13, bldg 2, Moscow
125412, Russia*

New emerging science is connected with formation of warm dense matter (WDM) at the initial transient state of material evolution after energy deposition into electron subsystem with electron temperatures T_e in the range 1-100 eV. Usually WDM forms in ultrafast phenomena and is a non-equilibrium state that makes it very challenging for theory, modelling and simulation (e.g. [1]). In many cases WDM can be described as a two-temperature (2T) system when electron and ion subsystems can be considered in quasi-equilibrium at $T_e > T_i$.

Both in continuum and in atomistic models it is assumed that the quasi-equilibrium 2T-WDM can be described using thermodynamic concepts. In this work on examples of Al and Au we are making an attempt to analyze the electronic contribution to the total pressure in 2T-WDM. Another question considered is the separation of electrons into bound and free.

We perform finite temperature Kohn-Sham density functional theory (FT KS DFT) calculations in the plane-wave basis. The electron-ion interaction for Al and Au is described by PAW potentials. We analyze the dependencies on the electronic temperature of the electronic pressure P_e components for fcc aluminum and gold for $T_e = 0-12$ eV. We see the strongest dependence on T_e in the kinetic and non-local pressure components. Using the pDOS-based analysis we decipher the bond hardening effect in fcc Au [2] as a transition of electrons from d-like states into s- and p-like states as well as into the plane-wave like (i.e. free) states.

We deploy the comparison of the Fermi gas model with the FT KS DFT results to understand the 2T-WDM properties better. We also consider the Hellmann-Feynman forces acting on ions in 2T-WDM. We are making the following conclusions [3].

The sum of kinetic and non-local DFT pressure components governs the build-up of the electron pressure in FT KS DFT models of warm dense metals. The non-local component of the electron-ion interaction plays an important role in the changes of warm dense metal properties with the increase of electronic temperature.

In the general case the increase of electron temperature in warm dense metal not only causes the free-electron pressure build-up, but also changes the effective interionic forces [1] and hence the binding pressure and the equation of state.

Using effective ion-ion potentials obtained by force-matching for different T_e [1] it is possible to separate the binding component of electron pressure and the free electron like component. This is a method (among several others [4]) for calculation of the number of free electrons, i.e. the ionization degree of WDM.

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