Energy relaxation and electron phonon coupling in laser heated solids

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A laser interacting with matter will leave the electrons in the target in an energetically enhanced state compared to the ions. A shock wave entering a system will heat the ions but leave the electrons in their ground state as before the shock wave. In any case, a non-equilibrium state is formed that will lead to a relaxation process towards a new thermodynamic equilibrium state. This relaxation is a multi stage process usually starting with the formation of an equilibrium electron distribution due to fast electron-electron collisions. Afterwards, the relaxation of the ionization state and the equilibration in between species take place along with the establishment of ion equilibrium momentum distributions.

Here, we focus on the special situation in which the conduction electrons in a metal have already established a high temperature in the electron volt range due to past optical laser irradiation and are significantly hotter than the lattice which, at the beginning of the modelling, is still at room temperature. Such a situation might be described using a two-temperature model (or by extension a multi-temperature model with different temperatures for different phonon modes). The energy transfer can be calculated by considering a set of Boltzmann equations for the electrons and different phonon modes. Important input quantities are the electronic density of states (DOS) $g(\varepsilon)$ and the occupation numbers of the electronic states $f(\varepsilon)$ in order to determine what the electronic states around the Fermi edge ε_F actually contribute to the energy transfer. The phonon states receiving the energy are determined by the phonon DOS and the electron-phonon coupling as incorporated in the Eliashberg function $\alpha^2F(\omega)$. The actual occupation of each phonon mode is given by the Bose distribution $n_B^p(\omega, T_p)$ [1, 2]

$$Z_{ep}(T_e, T_l, t) = \frac{2\pi N_c}{g(\varepsilon_F)} \int_{-\infty}^{\infty} d\varepsilon \, g^2(\varepsilon) \frac{\partial f_e(\varepsilon, T_e)}{\partial \varepsilon}$$

$$\times \int_0^{\infty} d\omega (\hbar\omega)^2 \alpha^2 F(\omega, T_e, T_l, t) \left[n_B^e(\omega, T_e) - n_B^p(\omega, T_p) \right].$$

The input quantities can be computed using density functional theory and the linear response formalism so that the lattice symmetries, ion-ion, electron-ion, and electron-electron correlations in a metal can be taken into account [3]. The electron-phonon coupling factor is then obtained from the energy transfer rate by dividing it by the temperature difference $G_{ep} = Z_{ep}/(T_e - T_p)$.

In Fig. 1, we show data for the electron-phonon coupling in copper with a fcc lattice structure. For these calculations, a stable lattice and DOS as at room temperature was assumed for all electron temperatures. The low temperature value of the electron-phonon coupling is in agreement with values given in Refs. [5, 6]. The values reported by Lin [4] are based on calculations by Savrasov et al. [7]. For higher electron temperatures, the obtained values are not in agreement with experimental results by Cho *et al.* and by Brown *et al.* [8, 9].

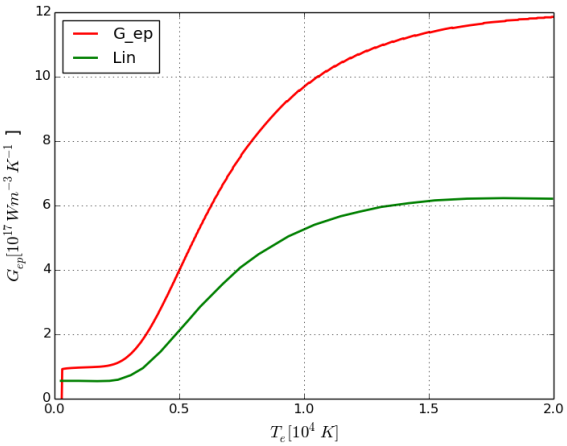

Figure 1: Electron-phonon coupling factor in fcc copper as a function of the electron temperature. The result of Lin *et al.* is taken vom Ref. [4].

Possible improvements in the theoretical description are the use of electronic DOS for the appropriate electron and ion temperatures as well as of temperature dependent electron-phonon coupling matrix elements.

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