Energy relaxation and electron-phonon coupling in laser-excited metals

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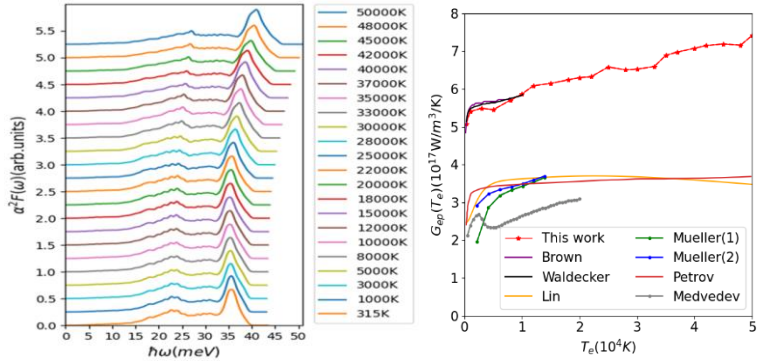
- **Motivation**: first-principles accurate determination of electron-phonon coupling factors for a wide variety of elements and materials are in high demand.
- **Formula**:

$$G_{ep}(T_e,T_l,t)=\frac{2\pi N_c}{g[\mu(T_e)](T_e-T_l)}\int_{-\infty}^{\infty}g^2(\varepsilon,T_e,T_l)\frac{\partial f(\varepsilon,T_e)}{\partial\varepsilon}d\varepsilon \times\int_0^{\infty}(\hbar\omega)^2\alpha^2F(\omega,T_e,T_l,t)[n_B^e(\omega,T_e,t)-n_B^p(\omega,T_l,t)]d\omega.$$

- **Scheme**:1)finite temperature DFT + tetrahedron method (to calculate T_e-dependent electron density of states). 2)finite temperature DFPT (to get the T_e-dependent Eliashberg function, unshifted k-point grid featuring 32 × 32 × 32 points and a subset thereof for the q-point grid of 8 × 8 × 8).

Electron-phonon coupling factor for simple metal Aluminum

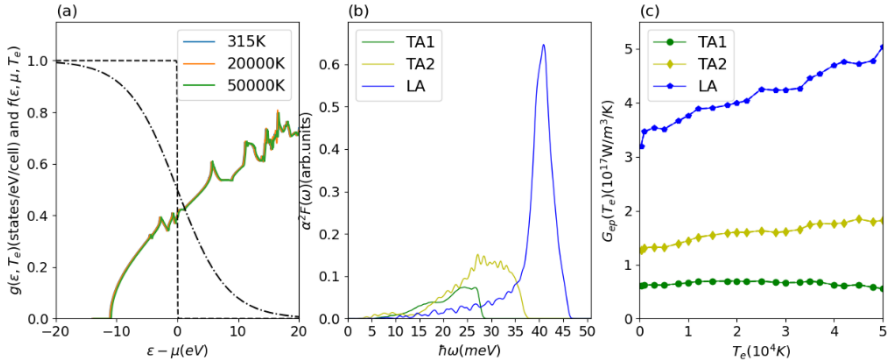
Broadening and shifting of spectral weights.



Coupling strength of longitudinal mode alone around 3.

Fig.1:Eliashberg function of Al at different electron temperatures.
Fig.2:electron temperature-dependent electron-phonon coupling factor of Al.

Little change with increasing electron temperature.



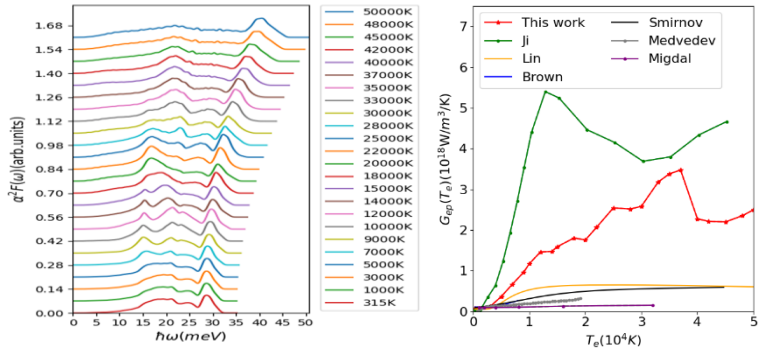
Longitudinal mode plays a dominant role.

Fig.3.: (a) electronic DOS of Al for different electron temperatures and Fermi distribution functions.(b) Eliashberg function of Al for three partial branches (TA1, TA2, LA) at Te=50000K and (c) electron temperature-dependent partial electron-phonon coupling factor of Al (TA1, TA2, LA).

➢ **we need the non-thermal lattice model,see Waldecker et al. PRX 2016.**

Electron-phonon coupling factor for transition metal Copper

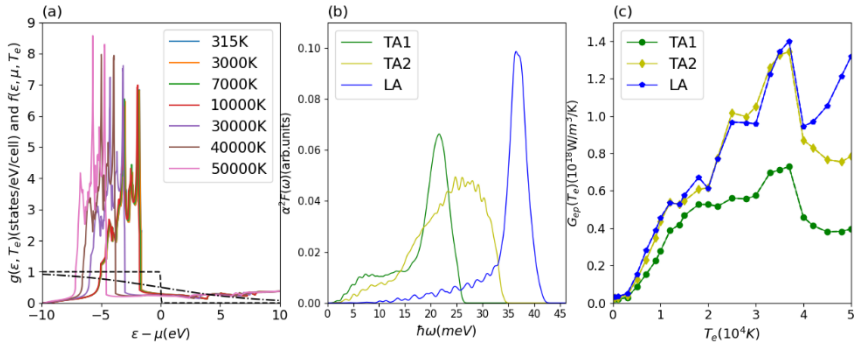
More complicated broadening and shifting behavior.



A characteristic dip at 37000K.

Fig.4:Eliashberg function of Cu at different electron temperatures.
Fig.5:electron temperature-dependent electron-phonon coupling factor of Cu.

Dramatic change under high electronic excitation.



No dominant partial mode.

Fig.6.: (a) electronic DOS of Cu for different electron temperatures and Fermi distribution functions.(b) Eliashberg function of Cu for three partial branches (TA1, TA2, LA) at Te=40000K and (c) electron temperature-dependent partial electron-phonon coupling factor of Cu (TA1, TA2, LA).

➢ **The two-temperature model should be valid (contrary to Al).**