***Ab initio* determination of effective electron-phonon coupling factor in copper**

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Abstract

The electron temperature T_e dependent electron density of states $g(\varepsilon)$, Fermi-Dirac distribution $f(\varepsilon)$, and electron-phonon spectral function $\alpha^2F(\Omega)$ are computed as prerequisites before achieving effective electron-phonon coupling factor G_{e-ph} . The obtained G_{e-ph} is implemented into a molecular dynamics (MD) and two-temperature model (TTM) coupled simulation of femtosecond laser heating. By monitoring temperature evolutions of electron and lattice subsystems, the result utilizing G_{e-ph} from *ab initio* calculation, shows a faster decrease of T_e and increase of T_l than those using G_{e-ph} from phenomenological treatment. The approach of calculating G_{e-ph} and its implementation into MD-TTM simulation is applicable to other metals.

Keywords: Electron-Phonon Interaction; Femtosecond Laser; Thin Film; Spectral Function

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1. Introduction

When a metallic system is under the conditions of neutron irradiation, swift heat ion and gamma radiation, as well as femtosecond laser heating, the electron temperature T_e , increases to tens of thousands of degrees Kelvin as a result of electron excitation. At a low lattice temperature T_l , the lattice subsystem remains unaffected. The large increase of T_e and relative cold T_l results in electron-phonon non-equilibrium. This strong non-equilibrium between the electron subsystem and lattice subsystem of a metal affects a large number of physical properties, such as the thermal conductivity, superconductivity and thermal stress propagation.

During the transport of the absorbed thermal energy from electron subsystem to lattice subsystem, the electron-phonon coupling factor G_{e-ph} , plays a crucial role in influencing the relaxation time needed to reach equilibration state. In the past 40 years, a large body of research has been performed to study electron-phonon interaction and thereby determine G_{e-ph} . The electron-phonon coupling constant λ_{const} was primarily proposed by Allen *et al.* [1, 2] to characterize the strength of electron-phonon coupling and was subsequently measured by using the pump-probe procedure [3]. Lin and Zhigilei proposed a T_e dependent G_{e-ph} and carried out related calculations by including the experimental $\lambda\langle\omega^2\rangle_{const}$ [4]. A phenomenological approach to calculating temperature dependent G_{e-ph} was derived by Chen *et al.* [5], which included both the effects of electron-electron and electron-phonon scattering. Many *ab initio* calculations were also performed to study G_{e-ph} [6–8]. Nevertheless, there is still no work that comprehensively treats all T_e dependent parameters (Fermi-Dirac distribution $f(\varepsilon)$, electron density of states $g(\varepsilon)$ and electron-phonon spectral function $\alpha^2F(\Omega)$) in obtaining G_{e-ph} .

This letter paves a new way of pure *ab initio* calculation of G_{e-ph} after derivation of all the essential parameters: $g(\varepsilon)$, $f(\varepsilon)$ and $\alpha^2 F(\Omega)$.

2. Computational details

Recalling the definition of G_{e-ph} , the effective electron-phonon coupling can be mathematically expressed by means of the rate of energy transportation $\partial E/\partial t$ per unit cell volume V_c at the temperature difference between T_e and T_l [2]

$$G_{e-ph} = \frac{\partial E}{\partial t} \frac{1}{T_e - T_l} \frac{1}{V_c} \quad (1)$$

When electrons are excited, the variations of $g(\varepsilon)$, $f(\varepsilon)$ and $\alpha^2 F(\Omega)$ from the room temperature contribute to $\partial E/\partial t$ between electron and lattice subsystems. By taking the electron-phonon collision into account, $\partial E/\partial t$ can be obtained as [2]

$$\frac{\partial E}{\partial t} = \frac{4\pi}{\hbar} \sum_{k, k'} \hbar \omega_Q |M_{k, k'}|^2 S(k, k') \delta(\varepsilon_k - \varepsilon_{k'} + \hbar \omega_Q) \quad (2)$$

where $\hbar$ is the reduced Planck constant 1.054×10^{-34} . k and k' are the electron quantum number at initial and final states, respectively. ω_Q denotes the phonon frequency at the phonon quantum number Q . The scattering probabilities of electrons at initial energy ε_k and final energy $\varepsilon_{k'}$ are described by the matrix $M_{k, k'}$. $S(k, k')$ equals $[(f_k - f_{k'})n_Q - f_{k'}(1 - f_k)]$, which is named as the thermal factor. f_k is the Fermi distribution function for electron, $1/[\exp(\frac{\varepsilon - \mu}{k_B T_e}) + 1]$. n_Q is the Bose distribution for phonon, $1/[\exp(\frac{\hbar \omega_Q}{k_B T_l}) - 1]$.

By introducing electron-phonon spectral function at a specified T_e

$$\alpha^2 F(\varepsilon, \varepsilon', \Omega)|_{T_e} = \frac{2}{\hbar g(\varepsilon_F)|_{T_e}} \sum_{k, k'} |M_{k, k'}|^2 \delta(\omega_Q - \Omega) \delta(\varepsilon_k - \varepsilon) \delta(\varepsilon_{k'} - \varepsilon') \quad (3)$$

and combining with Eq. (1) and (2), G_{e-ph} at specified T_e becomes

$$G_{e-ph}|_{T_e} = \frac{2\pi g(\varepsilon_F)|_{T_e}}{T_e - T_l} \frac{1}{V_c} \left\{ \int_0^\infty \left[\int_{-\infty}^\infty \left(\int_{-\infty}^\infty \alpha^2 F(\varepsilon, \varepsilon', \Omega) |_{T_e} d\varepsilon \right) \hbar \Omega d\Omega \right] S(\varepsilon, \varepsilon') |_{T_e} \delta(\varepsilon - \varepsilon' + \hbar \Omega) \right\} \quad (4)$$

The energy conservation requires that $\varepsilon' - \varepsilon = \hbar \Omega$, and the electron-phonon spectral function is approximated as [9]

$$\alpha^2 F(\varepsilon, \varepsilon', \Omega) |_{T_e} = g(\varepsilon) |_{T_e} g(\varepsilon + \hbar \Omega) |_{T_e} \alpha^2 F(\varepsilon_F, \varepsilon_F, \Omega) |_{T_e} / [g(\varepsilon_F) |_{T_e}]^2 \quad (5)$$

Moreover, at the limit of $k_B T_e \gg \hbar \Omega$ and $k_B T_l \gg \hbar \Omega$, the thermal factor becomes

$$S(\varepsilon, \varepsilon') |_{T_e} = [f(\varepsilon) - f(\varepsilon + \hbar \Omega)] (T_e - T_l) k_B / (\hbar \Omega) \quad (6)$$

Because the energy range of electrons is much wider than that of phonons, $g(\varepsilon)$ is approximately equal to $g(\varepsilon + \hbar \Omega)$ and $[f(\varepsilon) - f(\varepsilon + \hbar \Omega)] / (\hbar \Omega)$ in Eq. (6), which can be rewritten as $-\partial f / \partial \varepsilon$. In addition, at the high T_e limit, the second moment of $\alpha^2 F(\Omega) |_{T_e}$ is simplified as $\lambda \langle \omega^2 \rangle |_{T_e} = 2 \int_0^\infty \alpha^2 F(\Omega) |_{T_e} \Omega d\Omega$ [2] Therefore, Eq. (4) becomes

$$G_{e-ph}|_{T_e} = \frac{\pi \hbar k_B \lambda \langle \omega^2 \rangle |_{T_e}}{[g(\varepsilon_F) |_{T_e}]^2} \frac{1}{V_c} \int_{-\infty}^\infty [g(\varepsilon) |_{T_e}]^2 \left(-\frac{\partial f |_{T_e}}{\partial \varepsilon} \right) d\varepsilon \quad (7)$$

This letter focuses on the effective electron-phonon coupling factor of copper. The *ab initio* investigation of electron-phonon interaction is carried out by using the density function theory (DFT) code ABINIT [10]. The finite temperature density functional formalism proposed by Mermin [11] is utilized to represent the different degrees of electron excitation at given T_e . The thermalized electrons obey Fermi-Dirac distribution and are expressed at Kohn-Sham eigenstates in each self-consistent field calculation. The calculations are based on the local density approximation (LDA) in combining with the projector-augmented wave (PAW) atomic data [12] to obtain $g(\varepsilon)$ (shown in Fig. 1(a)) and $f(\varepsilon)$ (shown in Fig. 1(b)), and the norm-conserving pseudopotential method in cooperation with a linear response approach [13] to get

$\lambda\langle\omega^2\rangle$ at given T_e (shown in Fig. 2(c)). The linear response calculation of electron-phonon interaction is performed under the framework of the linear-muffin-tin-orbital (LMTO) method [14]. The valence electrons for copper are $3d^{10}4s^1$. After the convergence test, the Monkhorst-Pack k -points grid of $18 \times 18 \times 18$ and a cutoff energy of 32 Ha are chosen.

3. Results and discussion

The zero point of the horizontal axis in Fig. 1 is set as the Fermi energy ε_F . As seen in Fig. 1(a), as a result of the thermal excitation of the electron subsystem, $g(\varepsilon)$ at increased T_e presents the overall shift toward lower ε state. Figure 1(a) shows gradual shrinking of the d block, and similar d block changes were reported in [15,16]. The latter shrinkage is said to be due to a more attractive electron-ion potential as a result of a decrease in electronic screening of $3d$ block electrons. Additionally, with the left shift and shrinkage of $g(\varepsilon)$, its value slightly increases. The Fermi-Dirac distribution $f(\varepsilon)$ at T_e of 300 K , $1 \times 10^4 K$, $2 \times 10^4 K$ and $4 \times 10^4 K$ is shown in Fig. 1(b). When $T_e = 300 K$, it can be seen that $f(\varepsilon)$ focuses around the Fermi energy. With the continuously increasing T_e , $f(\varepsilon)$ gets smeared out. Some of the electrons at high T_e are thermally excited at ε above the Fermi energy ε_F . As seen in Fig. 1(b), when $f(\varepsilon) = 0.5$ at $T_e = 4 \times 10^4 K$, ε locates at the right side energy point of all the other three cases when $f(\varepsilon) = 0.5$, which indicates the increase of chemical potential μ at high T_e .

In order to present more detailed information of μ at high T_e , the result of $\mu - \varepsilon_F$ is plotted in Fig. 2(a). It can be seen that μ increases with increasing T_e . The result in Fig. 2(a) agrees with that shown in [15], which was obtained from *ab initio* calculation by using generalized gradient approximation (GGA) for exchange and correlation energy. The computed $g(\varepsilon_F)$ is shown in Fig. 2(b), which presents a gradually decreasing tendency with the increment of T_e . Since $g(\varepsilon_F)$

is the dominator in the right hand of Eq. (7), the gradually decreasing $g(\varepsilon_F)$ brings the positive impact to G_{e-ph} , which indicates that G_{e-ph} will be greater and greater under the continuous increment of T_e (assuming all the other T_e dependent parameters are kept as constants).

The electron-phonon spectral function $\alpha^2 F(\Omega)$ at given T_e is calculated from response linear calculation. For the purpose of comparison, the experimental result [3] and *ab initio* calculation result [13] are plotted in Fig. 3 together with T_e dependent $\alpha^2 F(\Omega)$ in the present work. The *ab initio* calculation result in [13] presents the highest peak when Ω is at 7 THz, which is not seen in the experimental result in [17] and all the results in present calculation in Fig. 3. It should be noted that $\alpha^2 F(\Omega)$ calculated in [13] did not take the finite temperature density functional theory into account. However, in the practical application of laser heating and neutron irradiation, the electron subsystem excites after photon energy deposition. For the experimental study of $\alpha^2 F(\Omega)$ by using the technique of forming tiny point contacts between copper and copper when electric voltage was added, the degree of electron excitation is unknown in the experiment [17]. Moreover, as seen in Fig. 3, frequency Ω locates from 0.8 THz to 9.6 THz, which indicates that the electron-phonon relaxation time is around the picosecond scale. With the continuous thermal excitation of the electron subsystem, main peaks of $\alpha^2 F(\Omega)$ (calculated in the present letter) shift toward the higher Ω region. Hence, it can be interpreted that the electron-phonon interaction becomes shorter at a higher degree of electron excitation. Accompanying the right shift of $\alpha^2 F(\Omega)$, the electron-phonon interaction value decreases after $T_e = 1.0 \times 10^4$ K; hence, a weaker electron-phonon interaction occurs at higher T_e .

On the basis of calculated $\alpha^2 F(\Omega)$, λ and $\lambda\langle\omega^2\rangle$ are computed to obtain G_{e-ph} in Eq. (7). Figure 2(c) shows the results of $\lambda\langle\omega^2\rangle$ at given T_e . When $T_e < 0.8 \times 10^4$ K, $\lambda\langle\omega^2\rangle$ is around

54 meV^2 . When T_e increases, $\lambda\langle\omega^2\rangle$ shows a peak (at $T_e = 1.4 \times 10^4 \text{ K}$) and decreases to 32 meV^2 when $T_e = 3.0 \times 10^4 \text{ K}$. Recalling $\lambda\langle\omega^2\rangle|_{T_e} = 2 \int_0^\infty \alpha^2 F(\Omega)|_{T_e} \Omega d\Omega$ and combining with Fig. 3, the peak of $\lambda\langle\omega^2\rangle|_{T_e=1.4 \times 10^4 \text{ K}}$ is mainly caused by slightly increasing $\alpha^2 F(\Omega)$ and a right shift of $\alpha^2 F(\Omega)$ toward high Ω . As a non-dimensional parameter quantitatively assessing the strength of electron-phonon interaction without taking Ω into consideration, λ is calculated and shown in Fig. 2(d). Almost similar profiles of $\lambda\langle\omega^2\rangle$ and λ are achieved in Figs. 2(c) and 2(d). However, after $T_e = 3.5 \times 10^4 \text{ K}$, λ shows lower value than that at $T_e = 3.5 \times 10^4 \text{ K}$. On the contrary, $\lambda\langle\omega^2\rangle$ shows the opposite trend induced by the right shift of $\alpha^2 F(\Omega)$, which helps to compensate for the continuous decrement of λ . Beaulac *et al.* [18] calculated λ as 0.116 and $\lambda\langle\omega^2\rangle$ as 44.897 meV^2 . The other *ab initio* linear response calculation result showed λ as 0.14 [13]. Brorson *et al.* [3] experimentally measured λ as 0.08 ± 0.01 and $\lambda\langle\omega^2\rangle$ as $29 \pm 4 \text{ meV}^2$ at $T_e = 590 \text{ K}$ by using the pump-probe approach. Even though the degree of electron excitation is unknown, all of these results [3, 13, 18] are in the ranges of λ and $\lambda\langle\omega^2\rangle$ variations of present results in Figs. 2(c) and 2(d), which verifies the T_e dependent λ and $\lambda\langle\omega^2\rangle$ calculated in this letter.

After obtaining the full set of $f|_{T_e}$, $g(\varepsilon)|_{T_e}$, $g(\varepsilon_F)|_{T_e}$ and $\lambda\langle\omega^2\rangle|_{T_e}$, the T_e dependent G_{e-ph} are calculated from Eq. (7). As seen in Fig. 2(e), G_{e-ph} (calculated in the present letter) firstly shows a steep increment to $5.6 \times 10^{18} \text{ W}/(\text{m}^3 \text{ K})$ at $T_e = 1.4 \times 10^4 \text{ K}$. The slight decrease of G_{e-ph} when $1.4 \times 10^4 \text{ K} < T_e \leq 3.0 \times 10^4 \text{ K}$ and increase when $T_e > 3.0 \times 10^4 \text{ K}$ disagree with the profiles of $\lambda\langle\omega^2\rangle$ and λ shown in Figs. 2(c) and 2(d). $\lambda\langle\omega^2\rangle|_{T_e=1.4 \times 10^4 \text{ K}}$ is 2.4 times of $\lambda\langle\omega^2\rangle|_{T_e=3.0 \times 10^4 \text{ K}}$, whereas, $G_{e-ph}|_{T_e=1.4 \times 10^4 \text{ K}}$ is only 1.5 times of $G_{e-ph}|_{3.0 \times 10^4 \text{ K}}$. Considering $g(\varepsilon_F)$ shown in Fig. 2(b), it can be concluded that the inverse of $g(\varepsilon_F)$ plays the

dominating role of slowing down the decrement of G_{e-ph} when $1.4 \times 10^4 K < T_e \leq 3.0 \times 10^4 K$. $g(\varepsilon_F)$ even facilitates the increment of G_{e-ph} when $T_e > 3.0 \times 10^4 K$. Compared with G_{e-ph} computed from treating $g(\varepsilon)$ and $\lambda\langle\omega^2\rangle$ as constants by Lin and Zhigilei, and Chen's phenomenological estimation [5] of $G_{e-ph} = G_0[A_e/B_l(T_e + T_l) + 1]$ (where $G_0 = 1.0 \times 10^{17} W/(m^3 K)$ [19], $A_e = 1.75 \times 10^7/(sK^2)$, $B_l = 1.98 \times 10^{11}/(sK)$ [20], and $T_l = 2835 K$ (the boiling point of copper)), the G_{e-ph} calculated in the present work shows great discrepancies. In Lin and Zhigilei's work [4], the effects of μ shift and g variation are both eliminated in calculating G_{e-ph} , which are two crucial parameters contribute to the increase of G_{e-ph} during electron excitation. In addition, the substitution of $\lambda\langle\omega^2\rangle = 29 \pm 4 meV^2$ from experimental result in [3] is also another limitation hindering the comprehensive accounting of the electron-phonon interaction induced by electron excitation. Even though Chen *et al.* [5] took both the contributions of T_e and T_l to G_{e-ph} into account by providing that $A_e(T_e + T_l) \ll B_l$, all the parameters G_0 , A_e and B_l are obtained from the experiments [19, 20]. It should be noted that before vaporization, the actual G_{e-ph} is lower than the result represented by the short dash line in Fig. 2(e). As explicitly seen in Fig. 2(e), when the electron temperature $T_e < 2 \times 10^3 K$, the *ab initio* determined G_{e-ph} is smaller than those treating $g(\varepsilon)$ and $\lambda\langle\omega^2\rangle$ as constants in calculating G_{e-ph} and phenomenological G_{e-ph} . Both the *ab initio* determined G_{e-ph} and constant $g(\varepsilon)$ and $\lambda\langle\omega^2\rangle$ calculated G_{e-ph} show that the effective electron-phonon coupling factor does not change with T_e . Whereas, the phenomenological G_{e-ph} presents monotonically increasing tendency with the increase of T_e . When $T_e > 1 \times 10^4 K$, the *ab initio* determined G_{e-ph} demonstrates almost 10 times of those treating $g(\varepsilon)$ and $\lambda\langle\omega^2\rangle$ as constants in calculating G_{e-ph} and phenomenological G_{e-ph} .

In order to test the impact of pure *ab initio* determined G_{e-ph} to the thermal energy transport from the electron subsystem to lattice subsystem, molecular dynamics (MD) and two-temperature model (TTM) coupled simulation is performed. The motion of copper atoms in the lattice subsystem is described by using MD, while the electron subsystem is characterized by a continuum energy equation in TTM. The embedded atom method (EAM) potential of copper [21] is chosen for its ability to represent the interatomic interaction. The lattice subsystem in MD and electron subsystem in TTM are coupled by G_{e-ph} . Detailed information of the MD-TTM coupled framework are seen elsewhere [22–25]. The laser pulse duration is set as 100 fs. The maximum intensity of laser pulse occurs at $t_0 = 15$ ps. The absorbed laser energy is set at 0.3 J/cm^2 . Optical penetration depth is chosen as 14.29 nm, for an incident laser with a laser wavelength of $\sim 320 \text{ nm}$ [26]. The entire simulation lasts for 30 ps, which contained the first 5 ps of room temperature control (in terms of canonical ensemble) to equilibrate the entire system and the second 5 ps of micro-canonical ensemble verification to check the equilibration of lattice and electron subsystems. The entire system is constructed with 578.3840 nm, 3.6149 nm and 3.6149 nm in x -, y - and z - directions. Two empty spaces with thicknesses of 173.5152 nm (occupying 30% of the entire length in x - direction) and 37.8384 nm (occupying 10 % of the entire length in x - direction) are set to allow the film (thickness: 347.0304 nm) to expand during and after laser irradiation.

Figure 4(a) shows the spatial distribution of T_e and T_l from MD-TTM coupled simulation by employing G_{e-ph} from *ab initio* calculation in the present letter. For comparison, Fig. 4(b) plots T_e and T_l calculated from MD-TTM coupled simulation by using the phenomenological G_{e-ph} [5]. Both T_l in the insets of Figs. 4(a) and 4(b) rise above the boiling point (2835 K) of copper. However, as seen from the starting points of T_l , no appreciable

thermal expansions occur in either case. Due to larger G_{e-ph} in Fig. 4(a) than that in Fig. 4(b), when the electrons are excited, larger amounts of thermal energy transfer from electron subsystem to lattice subsystem. This explains that why T_l is greater in the inset of Fig. 4(a) than that in the inset of Fig. 4(b) from 15 ps to 16 ps. As seen from T_l at 18 ps, after laser heating, the time taking for lattice subsystem to get equilibration in Fig. 4(a) is much shorter than that in Fig. 4(b). At 30 ps, T_l in the front side of the copper film is around 1,600 K in Fig. 4(a). Whereas, for the case of Fig. 4(b), T_l is around 1,200 K in the corresponding location of the copper film. In addition, it can be seen the lattice heated region locates $x < 0.44$ in Fig. 4(a). However, larger lattice heated region ($x < 0.52$) is found in Fig. 4(b). As for T_e , it can be seen that T_e in Fig. 4(a) presents smaller values than those in Fig. 4(b), which is mainly induced by greater G_{e-ph} in the case of Fig. 4(a) during electron excitation.

4. Conclusions

In summary, it is concluded that both the previous treatment of G_{e-ph} by using T_e independent $g(\varepsilon)$ and $\lambda\langle\omega^2\rangle$ in Eq. (7) [4] and the phenomenological G_{e-ph} [5] underestimate the effective electron-phonon interaction process. To take the variations of $g(\varepsilon)$, $f(\varepsilon)$ and $\alpha^2F(\Omega)$ during electron excitation are essential. The MD-TTM coupled simulation shows the results by utilizing pure *ab initio* calculated G_{e-ph} giving a shallower heated region and faster energy transfer (as a result of lower T_e and higher T_l) than those using phenomenological G_{e-ph} . Further experimental study is suggested to investigate and compare the results of laser heated copper film. The accurate determination of G_{e-ph} in the presented letter leaves no empirical G_{e-ph} in the MD-TTM coupled simulation and empowers the multi-scale modeling of laser material interaction.

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Figure Captions

Fig. 1 (a) Electron density of states and (b) Fermi-Dirac distribution for electrons at 300 K , 10,000 K , 20,000 K and 40,000 K .

Fig. 2 Electron temperature T_e dependent (a) relative chemical potential μ changes to Fermi energy ε_F , (b) electron density of states $g(\varepsilon)$ at the Fermi energy ε_F , (c) the second momentum of second moment of $\alpha^2 F(\Omega)$: $\lambda\langle\omega^2\rangle$, (d) the electron-phonon coupling factor λ , and (e) the effective electron-phonon coupling factor G_{e-ph} .

Fig. 3 Electron temperature T_e dependent electron-phonon spectral function. The experimental result and ab initio calculated result are from [3] and [13], respectively.

Fig. 4 Spatial distribution of electron temperature T_e and lattice temperature T_l from MD-TTM coupled simulation: (a) by using the electron-phonon coupling factor G_{e-ph} calculated by pure ab initio calculation in the present work (b) by using Chen's phenomenological G_{e-ph} [5].

Fig. 1

Fig. 2

Fig. 3

Fig. 4