Electron-phonon scattering and related electrical conductivity in noble and transition metals at high electron temperature

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Electrical conductivity of noble and transition metals due to the electron-phonon collisions is calculated in two-temperature state with hot electrons and ion temperature not exceeding the melting threshold. This state arises when the femtosecond laser pulse of the moderate intensity acts onto the metal surface. Calculated electrical resistivity shows reduction with the electron temperature increase in contrast to the ordinary growth of the electrical resistivity of metals with the increase of common temperature of electrons and ions in equilibrium state. This decrease of the electrical resistivity is more significant in the case of transition metals. Femtosecond laser pulse, two-temperature state, noble and transition metals, electrical resistivity, electron-phonon scattering

Introduction. When ultrashort (femtosecond) laser pulse acts onto the metal surface it causes first of all the increase of the electron temperature. Large difference between electron and ion masses retards the energy transfer from electrons to ions. That is why during some time interval the surface layer of matter irradiated by the laser pulse exists in two-temperature state with the high temperature of electrons T_e and smaller temperature of ions T_i [1]. For laser pulses of moderate intensities with the surface density of energy (fluence) taken up by the metal target up to 100 mJ/cm^2 electron temperature in the surface layer of a target reaches several eV [2]. At the same time the equalization of electron and ion temperatures may last several picosecond, during a time interval more long than the duration of the laser pulse. Elevated electron temperature results in the significant change of the kinetic transport characteristics of a metal which are due to the electron motion. The values of kinetic coefficients at high electron temperatures may to a great extent differ from that one at usual room temperature when the equilibrium between electrons and ions takes place. Increase of the electron temperature gives rise to the change of the electron-ion coupling coefficient $\alpha(T_e)$, which is responsible for the energy exchange between electrons and ions to give the energy transferred from electrons to ions per unit time as $\alpha(T_e)(T_e - T_i)$ [3, 4, 5]. Electron-phonon coupling determines the depth of the layer of a target heated by the laser action before the sensible change of the target volume together with the another kinetic parameter - electron heat conductivity coefficient. In metals under consideration heat propagates mainly by electrons. Both electron-ion and electron-electron collisions contribute to the heat conduction. The change of the frequency of electron-electron collisions with the electron temperature increase have been calculated in [6, 7]. Now we consider electron-phonon collisions and their contribution into the transport coefficients of metals in two-temperature state at high electron temperatures and ion temperatures not exceeding the melting threshold, namely electrical conductivity.

Electron-phonon relaxation times. As a targets for the femtosecond laser irradiation we take metals with the essential excitation of d-electrons at high electron temperatures arising in metal when heating the electron subsystem by irradiation. They are noble metals having at $T_e = 0$K completely filled d-band with the top separated from the Fermi level lying within the s-p-band by the energy interval not exceeding the value 1-2 eV which is of the order of the gap in many semiconductors (as an example we consider copper (Cu)). Another situation exists in transition metals in which the Fermi level occurs inside of d-band as well as inside of sp-band (we consider iron (Fe) to present transition metals). We use the kinetic equations for sp and d-electrons in the electric field [8] taking into account collisions of all these electrons with phonons to obtain within the τ-approach relaxation times τ_s and τ_d of respectively sp and d-electrons due to the electron-phonon scattering:

$$\tau_s(\varepsilon) = \frac{m_s/m_d H_{sd} + H_{dd} + G_{ds}}{(H_{ss} + H_{sd})(H_{dd} + G_{ds}) - H_{sd}H_{ds}} \tag{1}$$

$$\tau_d(\varepsilon) = \frac{m_d/m_s H_{ds} + H_{ss} + G_{sd}}{(H_{ss} + H_{sd})(H_{dd} + G_{ds}) - H_{sd}H_{ds}} \tag{2}$$

Expressions (1) and (2) define relaxation times of sp and d-electrons at those values of the electron energy when transition between sp and d-bands is possible. When the electron energy is sufficient only for sp-sp scattering, relaxation time of sp - electrons is simply

$$\tau_s(\varepsilon) = 1/H_{ss} \tag{3}$$

Here

$$H_{ss} = \int w(q)\frac{q^2}{2p^2}(2N_q + 1)\frac{2\pi}{p(2\pi\hbar)^3}m_s q dq \tag{4}$$

$$H_{sd} = \int w(q)\frac{p'}{p}\frac{p^2 + p'^2 - q^2}{2pp'}(2N_q + 1)\frac{2\pi}{p(2\pi\hbar)^3}m_d q dq \tag{5}$$

$$G_{sd} = \int w(q)(2N_q + 1)\frac{2\pi}{p(2\pi\hbar)^3}m_d q dq \tag{6}$$

Analogously

$$H_{dd} = \int w(q)\frac{q^2}{2p'^2}(2N_q + 1)\frac{2\pi}{p'(2\pi\hbar)^3}m_d q dq \tag{7}$$

$$H_{ds} = \int w(q)\frac{p}{p'}\frac{p^2 + p'^2 - q^2}{2pp'}(2N_q + 1)\frac{2\pi}{p'(2\pi\hbar)^3}m_s q dq \tag{8}$$

$$G_{ds} = \int w(q)(2N_q + 1)\frac{2\pi}{p'(2\pi\hbar)^3}m_s q dq. \tag{9}$$

m_s, m_d are respectively effective masses of sp and d-electrons. We use the parabolic approach of electron dispersion curves both in sp and d-bonds having different tops and effective masses to approximate electron density of states obtained from the density functional calculations. q is phonon quasimomentum,

$$N_q = \frac{1}{exp(\hbar\omega(q)/(kT_i)) - 1}$$

is a phonon distribution function at the temperature T_i ($\omega(q)$ - phonon frequency).

$$w_q = \frac{\pi q^2}{\omega}\left(\frac{4\pi Zne^2}{q^2\epsilon(q)}\right)^2$$

with n being the concentration of atoms, $\epsilon(q)$ - dielectric permittivity, Z is the effective charge of ion for its interaction with the electron through the screened Coulomn potential. p stands for the electron momentum in s-band, p' is the momentum of electron of d-band. When transition between sp and d-bands occurs as a result of electron-phonon interaction, p and p' are connected by the relation

$$p^2 - \frac{m_d}{m_s}p'^2 = 2m_s(\varepsilon_1 - \varepsilon_s),$$

where ε_s and ε_1 are bottom of sp and d-bands respectively.

By integrating over q in formulas (4-9) within the corresponding interval depending on the value of electron energy ε we obtain the relaxation times τ_s of sp and τ_d of d-electrons as functions of their energy. Then substituting them into the expressions for conductivity of sp and d-electrons

$$\sigma_s = \frac{2e^2}{3}\int\left(\frac{p}{m_s}\right)^2 \frac{1}{4kT_e cosh^2(\frac{\varepsilon-\mu}{kT_e})}\tau_s(\varepsilon)\frac{4\pi p^2 dp}{(2\pi\hbar)^3},$$

$$\sigma_d = \frac{2e^2}{3}\int\left(\frac{p'}{m_d}\right)^2 \frac{1}{4kT_e cosh^2(\frac{\varepsilon-\mu}{kT_e})}\tau_d(\varepsilon)\frac{4\pi p'^2 dp'}{(2\pi\hbar)^3},$$

we can calculate electrical conductivity and resistivity due to sp and d-electrons and total resistivity connected with the electron-phonon scattering.

Resistivity of copper and iron due to the electron-phonon collisions. Fig. shows results of calculation of the resistivity of noble metal copper as the function of electron temperature for two values of the ion temperature (300K and 1200 K), not exceeding the melting temperature.

More impressive fall of resistivity with the electron temperature growth exhibits iron, one of a sufficiently large group of transition metals. The dependence of iron resistivity on the electron temperature for the same values of temperature of ions (300K and 1200K) is presented in Fig. 2. The fall of resistivity of metals with conducting d-electrons at high electron temperatures can be explained by the reduction of electron scattering into the d-states because of the shift of the occupancy of electron energy states into high energy states and small phonon energy.

In addition in Fig. 3 results of calculation of Cu and Fe resistivity in dependence on the common for electrons and phonon temperature in equilibrium single temperature case are shown. Resistivity of metals under consideration in this case rises by the ordinary way as the temperature increases.

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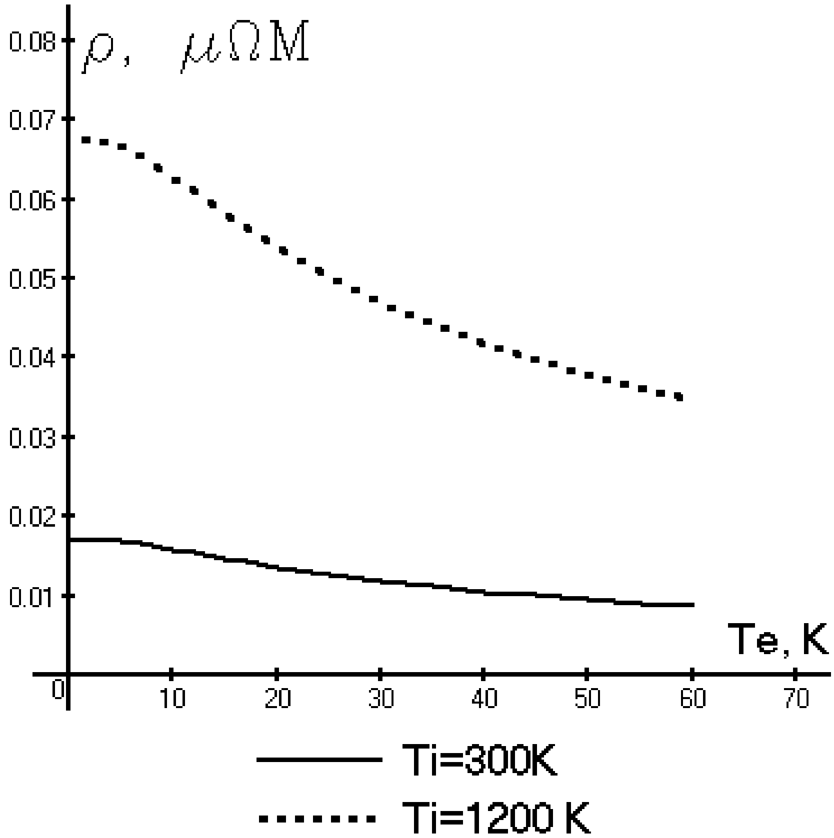

Figure 1: Electrical resistivity of copper at elevated temperature of electrons T_e for two values of the ion temperature 300K and 1200K. Resistivity drops with the electron temperature increase.

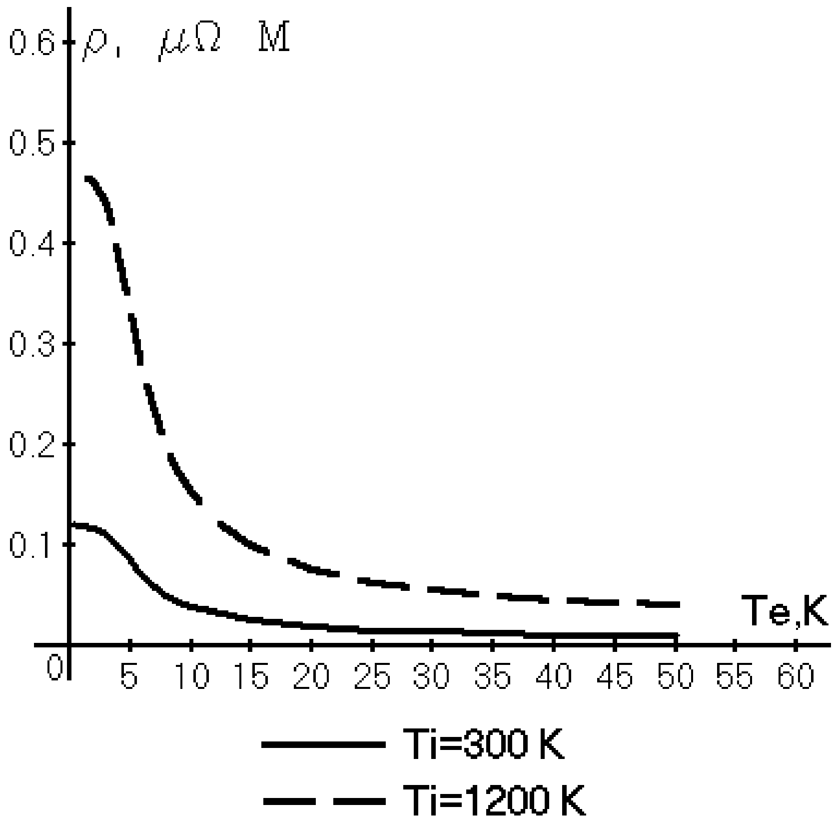

Figure 2: Resistivity of Fe in dependence on the temperature of electrons. It is obvious more significant drop of the electrical resistivity of iron than of copper in Fig. with the electron temperature increase. Ion temperature T_i takes the values 300K and 1200K.

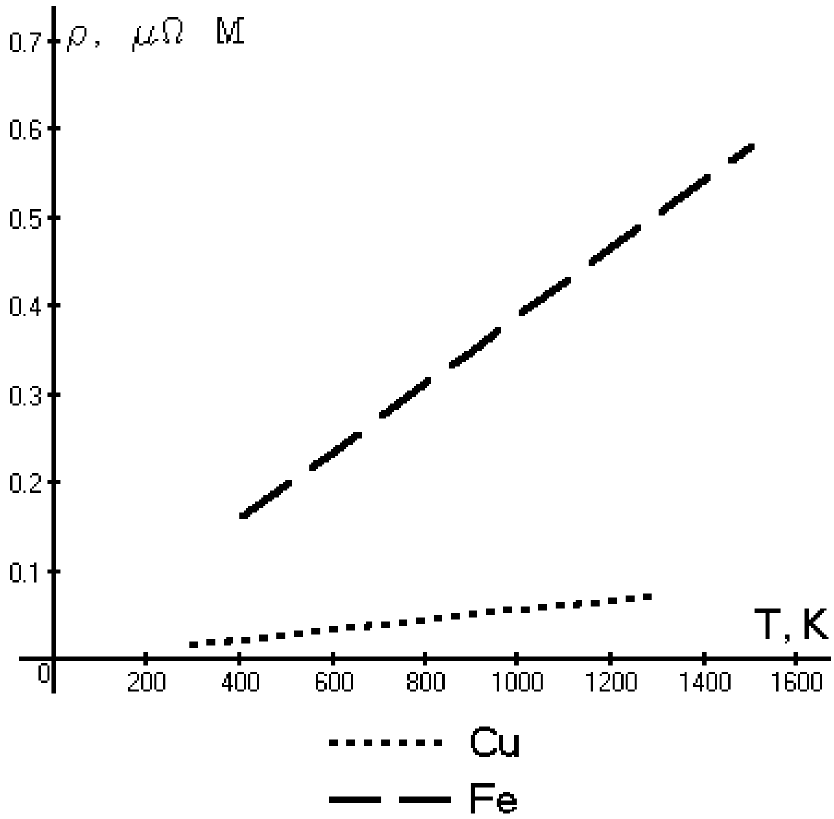

Figure 3: Calculated dependence of the resistivity of copper and iron due to the electron-phonon scattering upon the temperature of the metal in equilibrium case. Resistivity grows with the temperature increase.

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