THERMAL CONDUCTIVITY DUE TO S-S AND S-D ELECTRON INTERACTION IN NICKEL AT HIGH ELECTRON TEMPERATURES

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The essential feature of warm dense matter arising when ultrashort laser pulse acts on a metal target is a two-temperature state with hot electrons and cold crystalline lattice. Laser irradiation absorbed by a target initially heats a target within thin irradiation attenuation depth. Then heat propagates into the bulk target dominantly via the electron thermal conductivity being accompanied by the electron-ion energy exchange. In such a manner a target heated layer is produced. Because of ultrashort laser pulse duration and high speed of electron heat transfer the heated layer is formed practically with unchanged volume of a target. Depth of this heated layer and later dynamics of target expansion up to its ablation essentially depends upon the magnitude of electron thermal conductivity. For simple metals, such as aluminum, electron thermal conductivity coefficient was calculated in [1]. In transition metals (nickel as an example) there are two groups of electrons which affects the thermal conductivity caused by electrons. First of them are s- electrons with small effective mass, they have a high mobility and mainly contribute to the electron heat transfer. And the other group is d-electrons with much larger effective mass, and as a consequence their mobility and contribution to the heat flow is much smaller than for s-electrons. But d-electrons cause effective scattering of s-electrons in addition to s-s- scattering. We calculate the electron thermal conductivity coefficient and effective frequencies of s-s and s-d interactions in nickel at the wide range of electron temperatures when the thermal exitation of both s- and d-electrons is significant.

Consider the collision of s-electron having the momentum $\mathbf{p}$ with the electron having momentum $\mathbf{p\prime}$:

$$\mathbf{p}+\mathbf{p\prime} \longrightarrow (\mathbf{p}+\mathbf{q})+(\mathbf{p\prime}-\mathbf{q}) \tag{1}$$

Here $\mathbf{q}$ is a transferred momentum. Then the frequency of collisions of s-electron with the momentum $\mathbf{p}$ with other electrons can be written as

$$\nu(\mathbf{p}) = \frac{2\pi}{\hbar}\int\left(\frac{4\pi e^2}{\dfrac{q^2}{\hbar^2}+\varkappa^2}\right)^2 \frac{d^3q}{(2\pi\hbar)^3}\int\frac{2d^3p\prime}{(2\pi\hbar)^3}$$
$$\times\Phi(\mathbf{p},\mathbf{p\prime},\mathbf{q})\delta[\varepsilon(\mathbf{p})+\varepsilon\prime(\mathbf{p\prime})-\varepsilon(\mathbf{p}+\mathbf{q})-\varepsilon\prime(\mathbf{p\prime}-\mathbf{q})] \tag{2}$$

We suppose that the interaction between electrons has the screened Coulomn interaction form:

$$U(r) = \frac{e^2}{r}e^{-\varkappa r} \tag{3}$$

with the screening length $\lambda = \frac{1}{\varkappa}$. Statistical factor $\Phi(\mathbf{p},\mathbf{p\prime},\mathbf{q})$ is defined by the electron energy bands participating in the scattering process. Electron $ss \longrightarrow ss$ scattering is considered in [1] in detail.

When considering $ss \longrightarrow ss$ scattering, statistical factor has a form

$$\Phi(\mathbf{p},\mathbf{p\prime},\mathbf{q}) = f_s(\mathbf{p\prime})[1-f_s(\mathbf{p}+\mathbf{q})][1-f_s(\mathbf{p\prime}-\mathbf{q})]$$
$$+f_s(\mathbf{p}+\mathbf{q})f_s(\mathbf{p\prime}-\mathbf{q})[1-f_s(\mathbf{p\prime})], \tag{4}$$

where f_s is the Fermi function of s-electrons. Electron density of states of nickel at T=0K exibits strongly different s- and d-bands. We approximate s- and d-bands to be parabolic with effective masses of electrons consequantly $m_s = 1.1m, m_d = 7.7m$ (m is a free electon mass).

Now consider $s-d$ scattering as $sd \longrightarrow sd$ process and heat conductivity due to it. Electron energy in $s-$ and $d-$bands can be written as

$$\varepsilon(\mathbf{p}) = \varepsilon_s + \frac{p^2}{2m_s}, \qquad \varepsilon\prime(\mathbf{p\prime}) = \varepsilon_1 + \frac{\mathbf{p\prime}^2}{2m_d}, \tag{5}$$

where ε_s is a bottom of s-band, ε_1 is a bottom of d-band with a top of d-band to be ε_2. Statistical factor in this case is

$$\Phi(\mathbf{p},\mathbf{p\prime},\mathbf{q}) = f_d(\mathbf{p\prime})[1-f_s(\mathbf{p}+\mathbf{q})][1-f_d(\mathbf{p\prime}-\mathbf{q})]$$
$$+f_s(\mathbf{p}+\mathbf{q})f_d(\mathbf{p\prime}-\mathbf{q})[1-f_d(\mathbf{p\prime})] \tag{6}$$

Due to energy conservation

$$\varepsilon_s + \frac{(\mathbf{p}+\mathbf{q})^2}{2m_s} + \varepsilon_1 + \frac{(\mathbf{p\prime}-\mathbf{q})^2}{2m_d} = \varepsilon_s + \frac{p^2}{2m_s} + \varepsilon_1 + \frac{p\prime^2}{2m_d} \tag{7}$$

Denoting

$$\alpha = \frac{p^2}{2m_s} - \frac{(\mathbf{p}+\mathbf{q})^2}{2m_s}, \qquad \beta = \frac{(\mathbf{p\prime}-\mathbf{q})^2}{2m_d} - \frac{p\prime^2}{2m_d} \tag{8}$$

and also

$$\varepsilon = \frac{p^2}{2m_s}, \qquad \varepsilon\prime = \frac{p\prime^2}{2m_d}, \tag{9}$$

we obtain

$$\frac{(\mathbf{p}+\mathbf{q})^2}{2m_s} = \varepsilon - \alpha,$$

$$\frac{(\mathbf{p\prime}-\mathbf{q})^2}{2m_d} = \varepsilon\prime + \beta$$

Then statistical factor takes a form

$$\Phi(\alpha,\beta) = f_d(\varepsilon\prime)[1-f_s(\varepsilon-\alpha)][1-f_d(\varepsilon\prime+\beta)]$$
$$+f_s(\varepsilon-\alpha)f_d(\varepsilon\prime+\beta)[1-f_d(\varepsilon\prime)]. \tag{10}$$

Here at given electron temperature T

$$f_s(\varepsilon) = \frac{1}{e^{\dfrac{\varepsilon_s+\varepsilon-\mu}{kT}}+1}$$

$$f_d(\varepsilon) = \frac{1}{e^{\frac{\varepsilon_1 + \varepsilon - \mu}{kT}} + 1}$$

according to the suggestion of local thermal equilibrium in the electron subsystem. k is the Boltzmann constant. Then in terms of α and β

$$\Phi(\alpha,\beta) = \frac{e^{\frac{\varepsilon_1 + \varepsilon\prime - \mu}{kT}}}{e^{\frac{\varepsilon_1 + \varepsilon\prime - \mu}{kT}} + 1}$$

$$\times \frac{e^{\frac{\varepsilon_s + \varepsilon + \beta - \alpha - \mu}{kT}} + 1}{\left(e^{\frac{\varepsilon_s + \varepsilon - \alpha - \mu}{kT}} + 1\right)\left(e^{\frac{\varepsilon_1 + \varepsilon\prime + \beta - \mu}{kT}} + 1\right)} \tag{11}$$

Now δ-function responsible for energy conservation has a form $\delta(\alpha-\beta)$ and the collision frequency of s-electrin having the momentum $\mathbf{p}$ with d-electrons can be performed as

$$\nu(\mathbf{p}) = \nu(p) = \tfrac{2\pi}{\hbar}\int \left(\frac{4\pi e^2\hbar^2}{q^2 + \varkappa^2\hbar^2}\right)^2 \frac{d^3q}{(2\pi\hbar)^3}\frac{2d^3p\prime}{(2\pi\hbar)^3}$$
$$\times\Phi(\alpha,\beta)\delta(\alpha-\beta) \tag{12}$$

Introducing polar and azimuthal angles ϑ, φ for vector $\mathbf{q}$ (ϑ is the angle between $\mathbf{p}$ and $\mathbf{q}$), we can write

$$d^3q = 2\pi q^2 dq dt$$

Here $t = -cos(\vartheta)$ and we have integrated the q-space volume element over the azimuthal angle φ from 0 to 2π. With a new variable t

$$\alpha = \frac{p^2 - (\mathbf{p}+\mathbf{q})^2}{2m_s} = \frac{2pqt - q^2}{2m_s}$$

Then we obtain:

$$dt = \frac{m_s}{pq}d\alpha$$

At given $\mathbf{q}$ we can introduce polar and azimuthal angles $\vartheta\prime, \varphi\prime$ for the vector $\mathbf{p}\prime$ ($\vartheta\prime$ is the angle between $\mathbf{p}\prime$ and $\mathbf{q}$) Then

$$d^3p\prime = 2\pi p\prime^2 dp\prime dt\prime$$

Again $d^3p\prime$ is integrated over $\varphi\prime$ from 0 to 2π. Now we can write β in the form

$$\beta = \frac{(\mathbf{p}\prime - \mathbf{q})^2 - \mathbf{p}\prime^2}{2m_d} = \frac{2p\prime qt\prime + q^2}{2m_d}$$

and

$$dt\prime = \frac{m_d}{p\prime q}d\beta$$

Then we obtain

$$\frac{d^3q}{(2\pi\hbar)^3}\frac{2d^3p\prime}{(2\pi\hbar)^3}\Phi(\alpha,\beta)\delta(\alpha-\beta)$$

$$= \frac{dq}{(2\pi\hbar)^3}\frac{2dp\prime}{(2\pi\hbar)^3}\frac{2\pi m_s}{p}2\pi m_d p\prime d\alpha\; d\beta\Phi(\alpha,\beta)\delta(\alpha-\beta)$$

After the integration over β because of the presence of δ-function this expression is transformed to

$$\frac{dq}{(2\pi\hbar)^3}\frac{2dp\prime}{(2\pi\hbar)^3}\frac{2\pi m_s}{p}2\pi m_d p\prime d\alpha\Phi(\alpha,\alpha),$$

where statistical factor has the form

$$\Phi(\alpha,\alpha) = \frac{e^{\frac{\varepsilon_1 + \varepsilon\prime - \mu}{kT}}}{e^{\frac{\varepsilon_1 + \varepsilon\prime - \mu}{kT}} + 1}$$

$$\times \frac{e^{\frac{\varepsilon_s + \varepsilon - \mu}{kT}} + 1}{\left(e^{\frac{\varepsilon_s + \varepsilon - \alpha - \mu}{kT}} + 1\right)\left(e^{\frac{\varepsilon_1 + \varepsilon\prime + \alpha - \mu}{kT}} + 1\right)}.$$

Let calculate the integral over α

$$\int_{\alpha'}^{\alpha''}\Phi(\alpha,\alpha)d\alpha = \frac{e^{\frac{\varepsilon_1 + \varepsilon\prime - \mu}{kT}}\left(e^{\frac{\varepsilon_s + \varepsilon - \mu}{kT}} + 1\right)}{e^{\frac{\varepsilon_1 + \varepsilon\prime - \mu}{kT}} + 1}$$

$$\times \frac{kT}{e^{\frac{\varepsilon_1 + \varepsilon\prime - \mu}{kT}} e^{\frac{\varepsilon_s + \varepsilon - \mu}{kT}} - 1} \ln \frac{e^{\frac{\alpha}{kT}} + e^{-\frac{\varepsilon_1 + \varepsilon\prime - \mu}{kT}}}{e^{\frac{\alpha}{kT}} + e^{\frac{\varepsilon_s + \varepsilon - \mu}{kT}}}$$

$$= \tilde{\Phi}(\alpha', \alpha'')$$

Because of after scattering d-electron remains in d-band, it means that

$$\varepsilon_1 \leqslant \varepsilon_1 + \frac{(\mathbf{p}\prime - \mathbf{q})^2}{2m_d} \leqslant \varepsilon_2$$

$$\frac{p\prime^2 + 2p\prime qt\prime + q^2}{2m_d} \leqslant \varepsilon_2 - \varepsilon_1$$

Let us introduce the boundary momentum of d-electrons $p_d = \sqrt{2m_d(\varepsilon_2 - \varepsilon_1)}$ Then $p \leqslant p_d$ and $p\prime^2 + 2p\prime qt\prime + q^2 \leqslant p_d^2$ It follows from here that $t\prime \leqslant \frac{p_d^2 - p\prime^2 - q^2}{2p\prime q} = t_0$ In dependence of position of point t_0 with respect to the interval $[-1, 1]$ two cases arise. Case I: $t_0 \geqslant 1$. In this case integratioin over $t\prime$ is made within the interval $[-1, 1]$. In a case II $1 \leqslant t_0 \leqslant 1$ and we integrate over $t\prime$ in limits $1 \leqslant t\prime \leqslant t_0$. Considering all variants when integration over β gives different from zero result because of the presence of $\delta(\alpha - \beta)$ in equation (12), we obtain different regions of two-dimensional integration in $p\prime - q$ plane at given p as

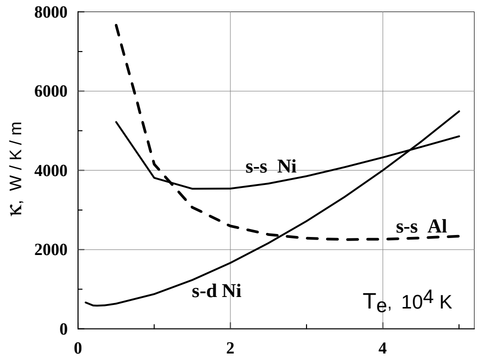

Figure 1. Electron thermal conductivity coefficient due to s-s and s-d scattering in nickel as compared with that one in aluminum (in aluminum only s-s scattering contributes to the electron thermal conductivity).

a parameter. Making an integration over $p\prime$ and q, we thus obtain the collision frequency $\nu(p)$ at given p.

Then we can obtain the thermal conductivity coefficient due to s-d electron scattering :

$$\varkappa_{sd}(T) = \frac{k}{3}\int(\varepsilon-\mu)\left(-\frac{\partial f_s}{\partial\varepsilon}(\varepsilon)\right)\left(\frac{\partial\mu}{\partial T}+\frac{\varepsilon-\mu}{T}\right) \times\frac{v_s^2(p)}{\nu(p)}\frac{p^2dp}{\pi^2\hbar^3}. \tag{13}$$

Here v_s is a velocity of s-electrons. From calculated values $\varkappa_{sd}(T)$ we can also define an average frequency of s-d electron collisions $\bar{\nu}_{sd}(T)$ using the Drude relation with the average squared velocity of s-electrons and their heat capacity per unit volume $C_s(T)$:

$$\varkappa_{sd}(T) = \frac{1}{3}\frac{C_s(T)\bar{v}_s^2}{\bar{\nu}_{sd}(T)} \tag{14}$$

Calculated thermal conductivity coefficient due to s-s and s-d electron scattering in nickel as a function of electron temperature is shown in Fig.1 in comparison with that one in aluminum. In aluminum only s-s electron scattering contributes to the electron thermal conductivity. Average frequency of s-s and s-d electron collisions deduced from the expression (14) is displayed in Fig. 2 for both materials. Within the electron temperature interval of the order of several eV of these frequencies under consideration s-d collision frequency in nickel exibits nonmonotonic behaviour. Electron-electron collision frequency together with the frequency of electron-ion collisions define total electron relaxation responsible for the electron thermal conductivity.

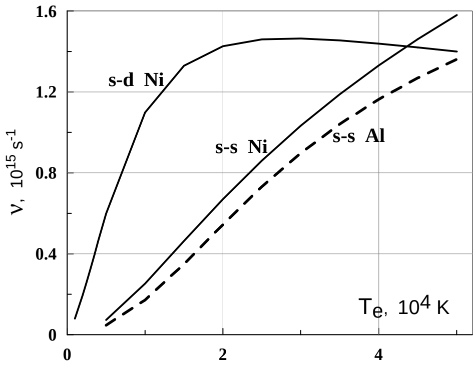

Figure 2. Electron-electron collision frequency in nickel because of s-s and s-d scattering and frequency of s-s electron collisions in aluminum.

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1. Inogamov N. A., Petrov Yu. V. // JETP 2010. V. 110. No. 3. P. 446.