Ю.В. Петров, С.И. Анисимов, Н.А. Иногамов, В.А. Хохлов, К.П. Мигдал.

Электропроводность и теплопроводность металлов при высоких электронных температурах, возникающих при воздействии на них фемтосекундных лазерных импульсов.

Two-temperature hydrodynamics approach

$$\rho^0 \frac{\partial u}{\partial t} = -\frac{\partial p}{\partial x^0}$$

$$\rho^0 \frac{\partial (E_e/\rho)}{\partial t} = \frac{\partial}{\partial x^0}\left(\frac{\rho\kappa}{\rho^0}\frac{\partial T_e}{\partial x^0}\right) - p_e \frac{\partial u}{\partial x^0} - \frac{\rho^0}{\rho}\alpha(T_e - T_i) + \frac{\rho^0}{\rho} Q$$

$$\rho^0 \frac{\partial (E_i/\rho)}{\partial t} = p_i \frac{\partial u}{\partial x^0} + \frac{\rho^0}{\rho}\alpha(T_e - T_i)$$

Hydrodynamics equations describe:

Heating of ion subsystem via energy transfer from hot electrons to ions (term with the coefficient α)

Expansion of electron thermal wave into the bulk target (the κ - term – electron heat conduction in the equation for the energy of electrons)

Expansion of a hot target matter

Коэффициент теплопроводности

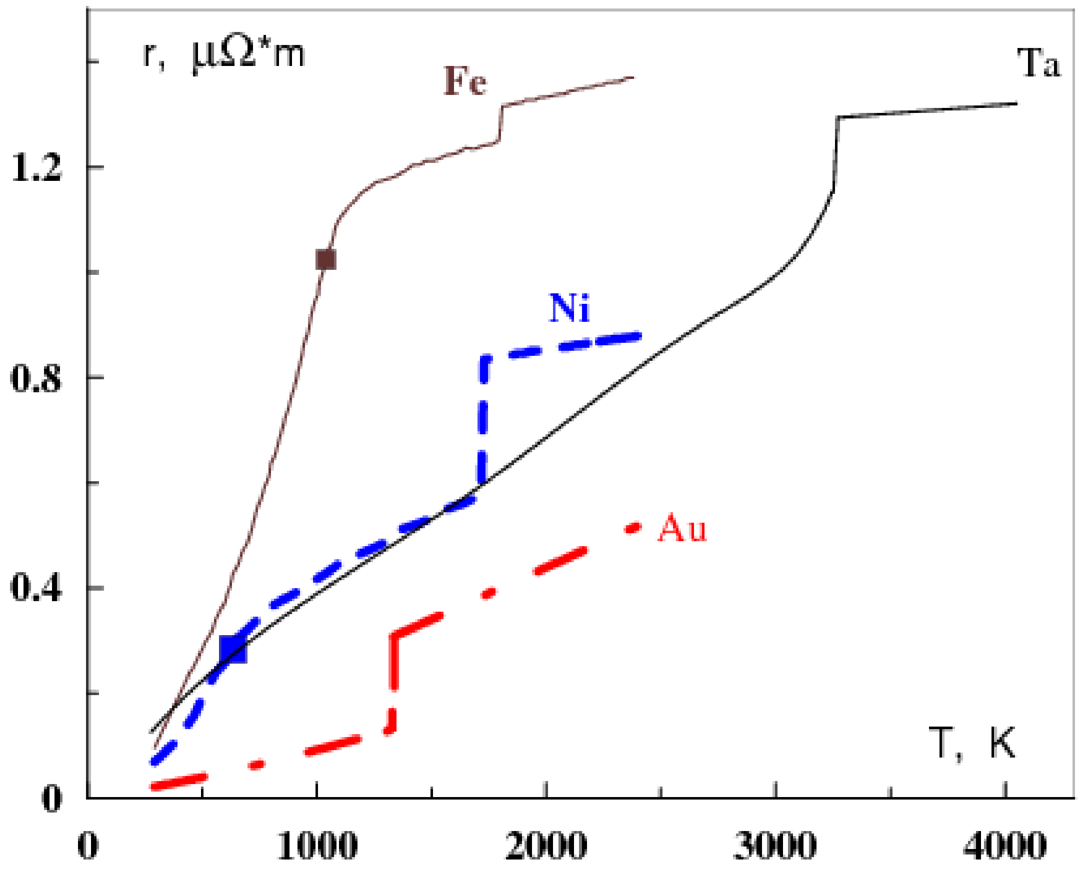
$$\kappa = \frac{1}{3}\int \left(\frac{\varepsilon - \mu}{T_e} + \frac{\partial \mu}{\partial T_e} \right) \frac{(\varepsilon - \mu)\mathrm{v}^2}{\nu(p)} \left(-\frac{\partial f}{\partial \varepsilon} \right) \frac{p^2 dp}{\pi^2 \hbar^3}$$

Проводимость

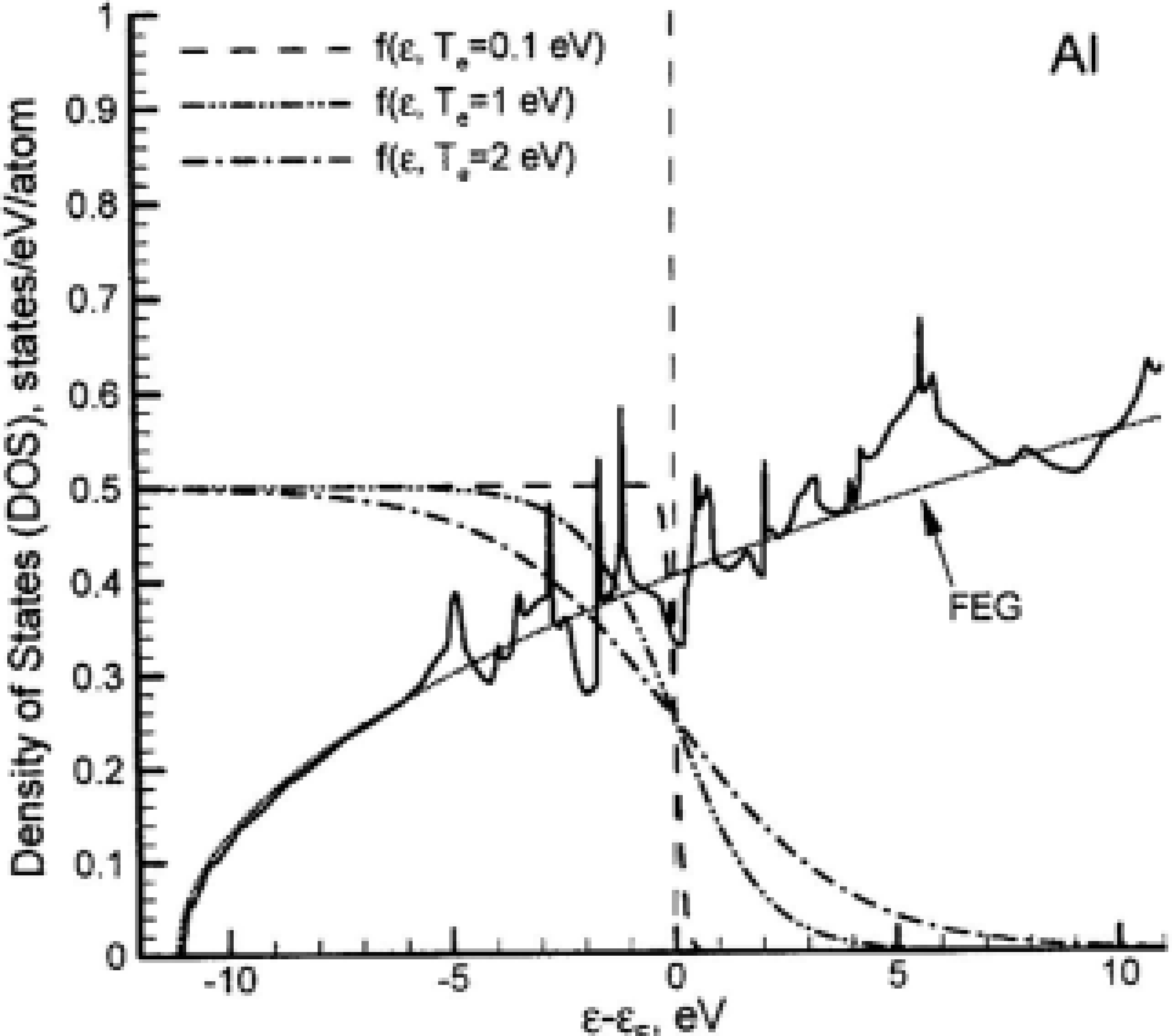
$$\sigma = \frac{1}{3} e^2 \int \frac{\mathrm{v}^2}{\nu(p)} \left(-\frac{\partial f}{\partial \varepsilon} \right) \frac{p^2 dp}{\pi^2 \hbar^3}$$

$$\nu \to \nu_{ei}, \nu_{ee}$$

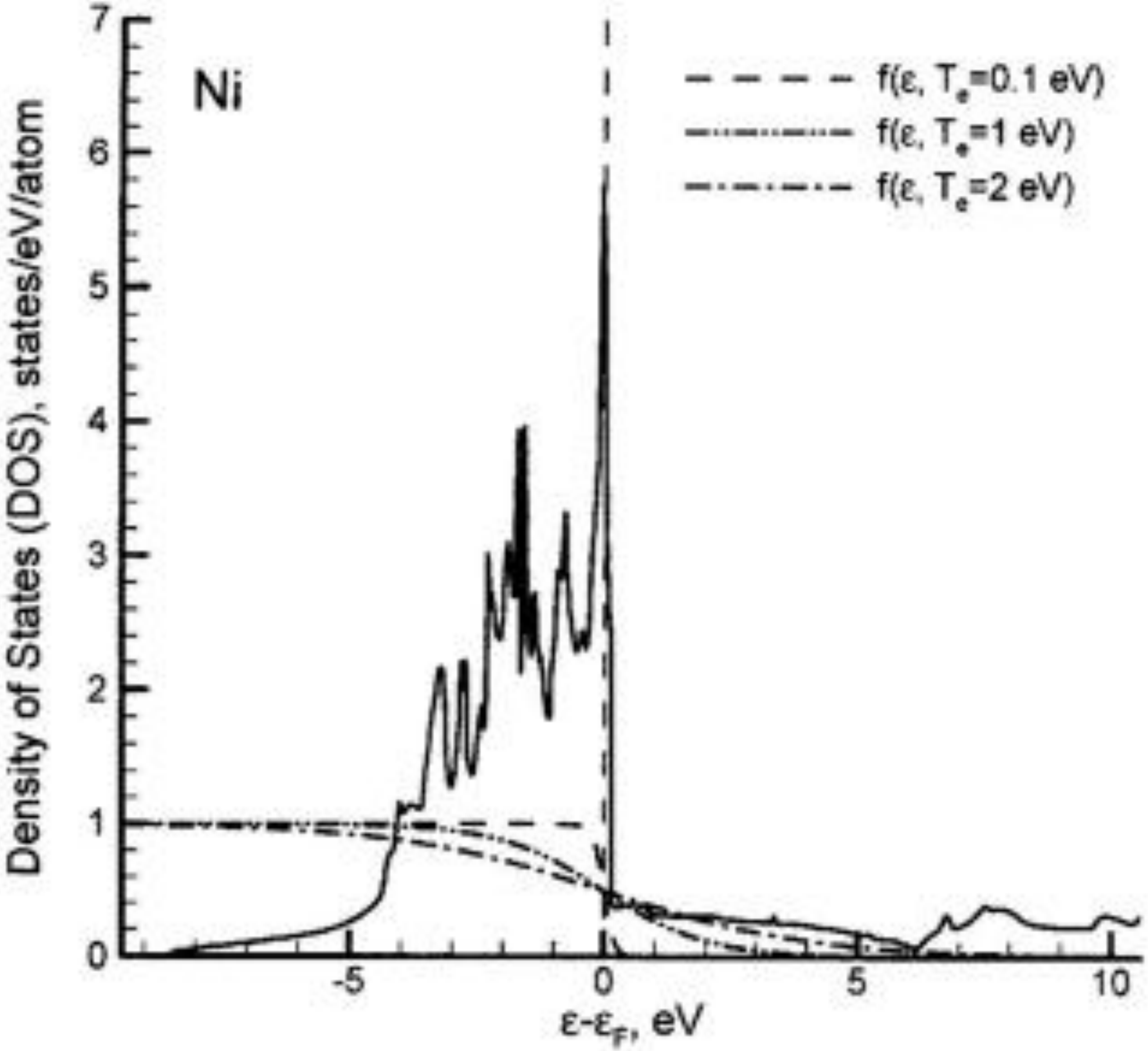
Удельное сопротивление некоторых металлов в равновесном случае



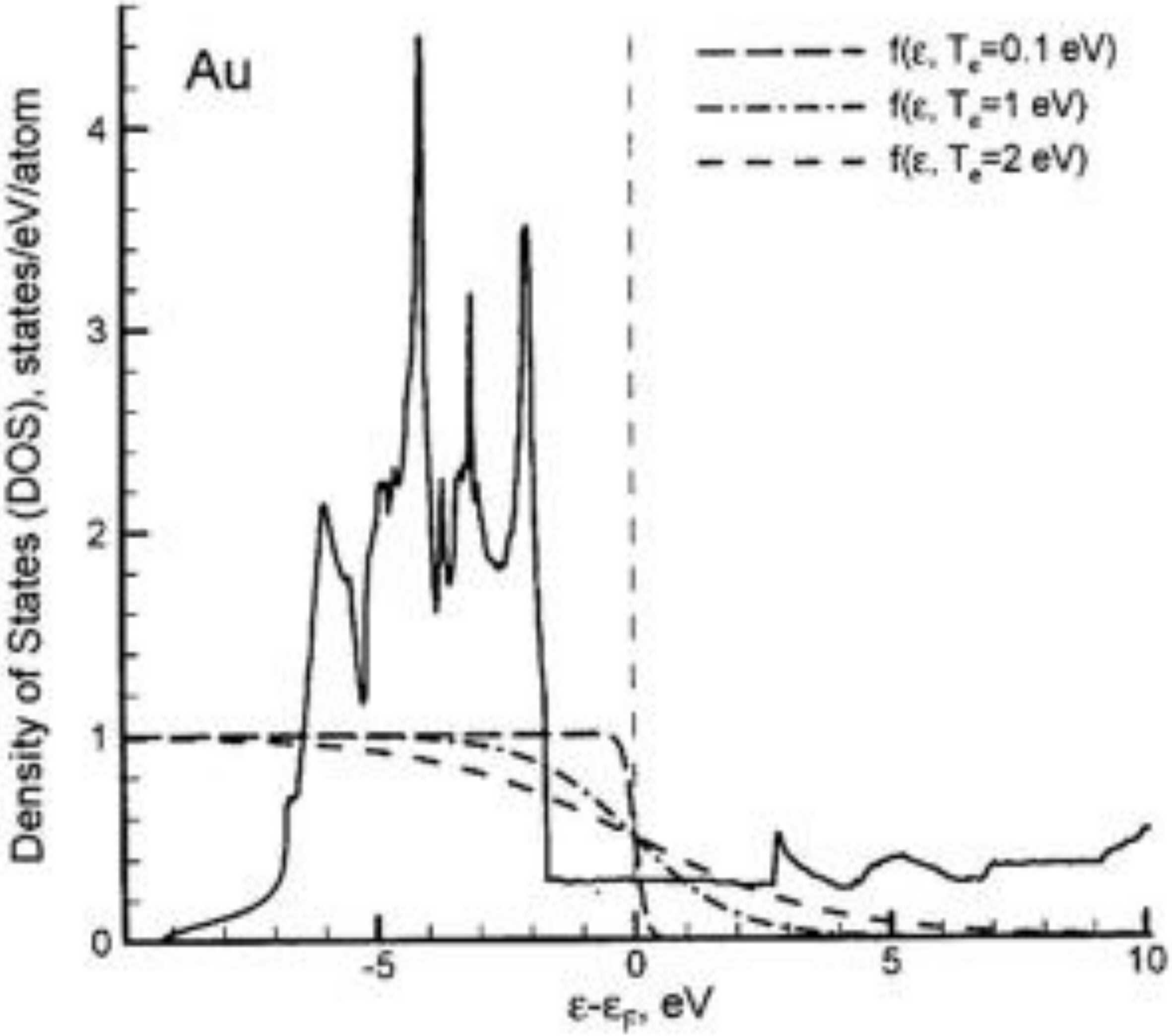
Al electron density of states



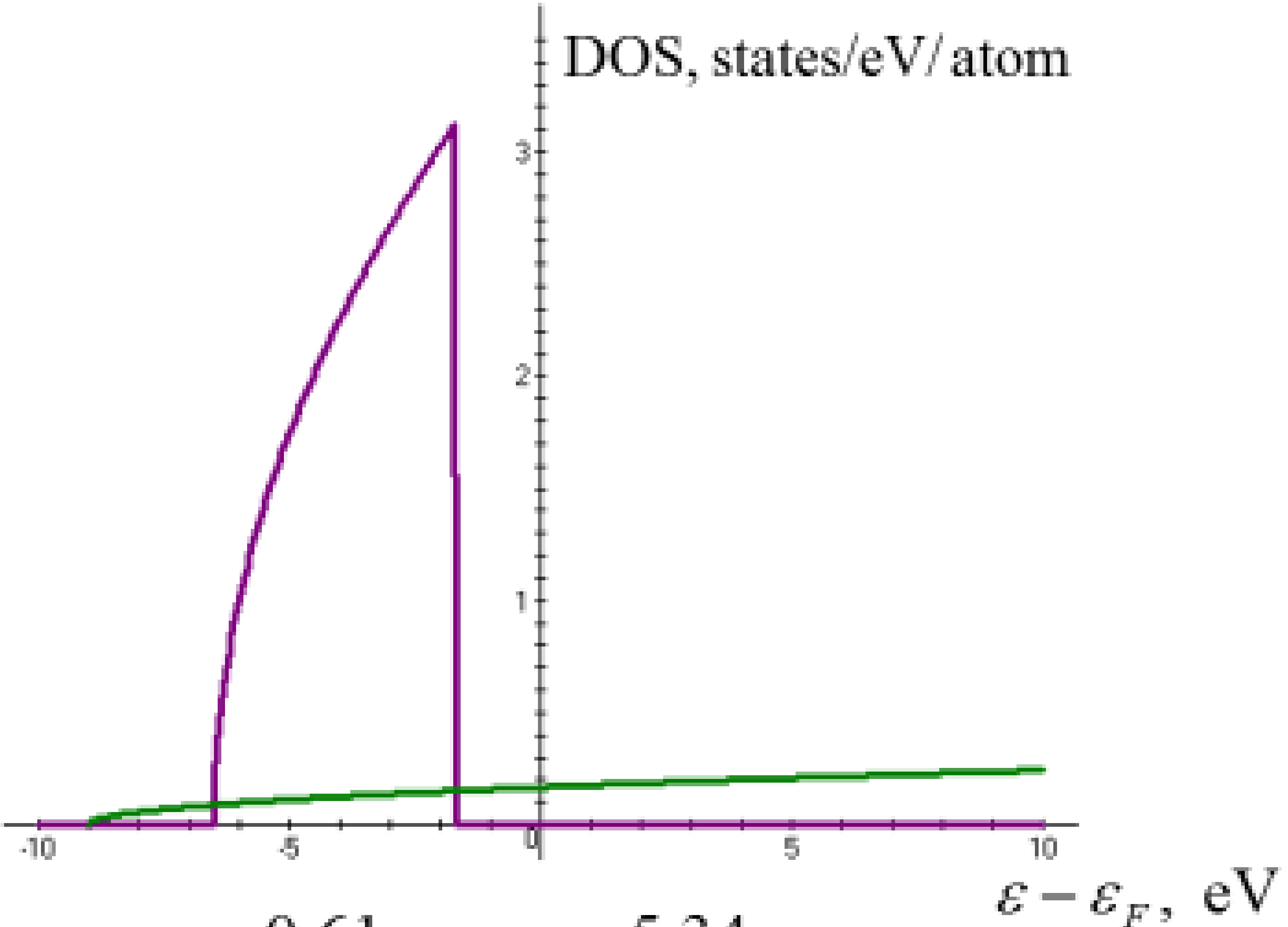
Ni electron density of states



Au electron density of states



Parabolic approximation of Au density of states (DOS)



$m_s = 0.61 \qquad m_d = 5.34$

Электрон-фононное рассеяние

Система кинетических уравнений для s- и d-электронов

$$(H_{ss}+G_{sd})\tau_s-\frac{m_s}{m_d}H_{sd}\tau_d=1$$

$$\frac{m_d}{m_s}H_{ds}\tau_s-(H_{dd}+G_{ds})\tau_d=-1$$

Отсюда

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

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

Матричные элементы

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

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

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

$$\frac{p^2}{2m_s(\varepsilon_1-\varepsilon_s)}-\frac{p'^2}{2m_d(\varepsilon_1-\varepsilon_s)}=1$$

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

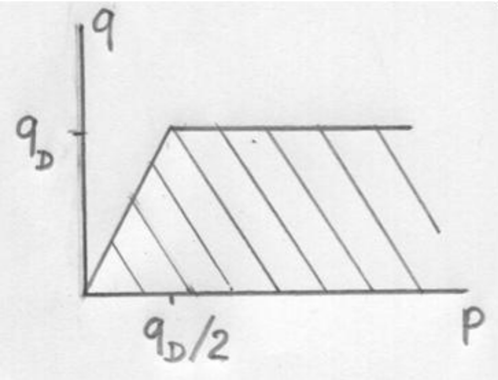
$$H_{ds}(p)=\int w(q)\frac{p}{p'}\frac{p^2+p'^2-q^2}{2pp'}(2N_q+1)\frac{V}{(2\pi\hbar)^3}\frac{2\pi}{p'}m_d q dq$$

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

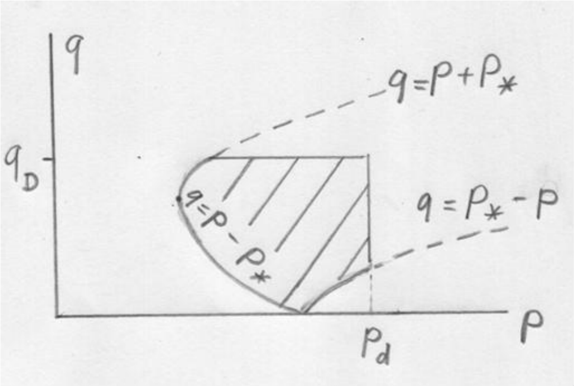
$$w(q)=\frac{\pi}{\rho V\omega(q)}q^2\left(\frac{4\pi z n e^2}{q^2\varepsilon(q)}\right)^2$$

Области интегрирования на плоскости p-q

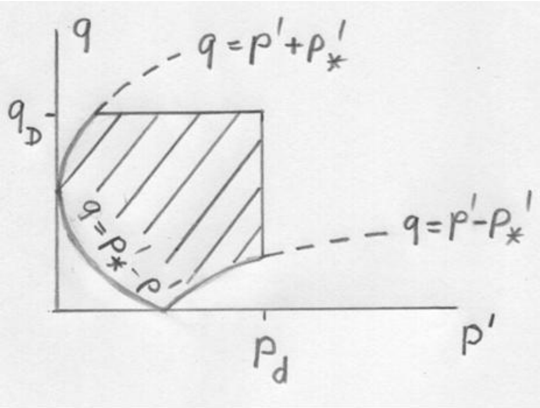
s-s



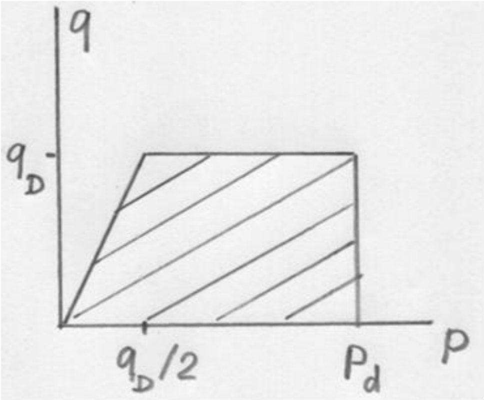
s-d



d-s



d-d

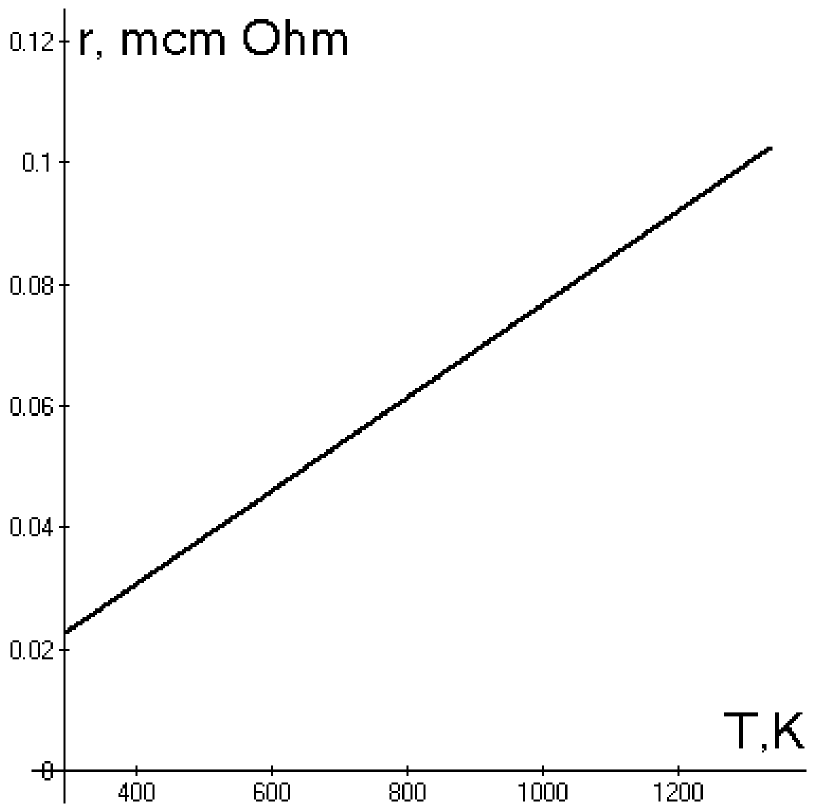


$$p'_*(p) = \sqrt{2m_s\left(\varepsilon_1 - \varepsilon_s + p'^2/2m_d\right)}$$

$$p_*(p) = \sqrt{2m_d\left(\varepsilon_s - \varepsilon_1 + p^2/2m_s\right)}$$

ε_s, ε_1 - уровни дна s- и d-зон

Удельное сопротивление золота в равновесном случае



Effective frequency of s-d electron-electron collisions

Scatterng of electrons with momentum $\mathbf{p}$ and $\mathbf{p}'$

and transferred momentum $\mathbf{q}$

$$\mathbf{p} + \mathbf{p}' \rightarrow (\mathbf{p} + \mathbf{q}) + (\mathbf{p}' - \mathbf{q})$$

Electrons interact through the screened Coulomb interaction

$$U(r) = \frac{e^2}{r} e^{-\kappa r}$$

with a screening length

$$\lambda = \frac{1}{\kappa}$$

Frequency of collisions of s-electron with momentum $\mathbf{p}$ with other electrons

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

$\Phi(\mathbf{p},\mathbf{p}',\mathbf{q})$ is a statistical factor

When considering sd->sd scattering

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

At electron temperature T Fermi functions are

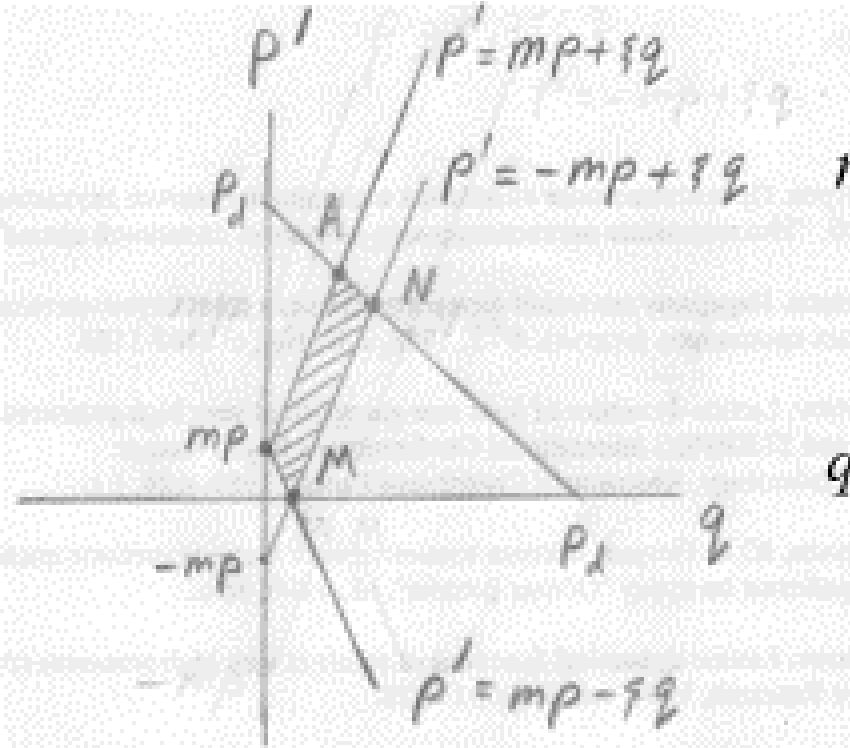
$$f_s(\varepsilon) = \frac{1}{e^{\frac{\varepsilon_s + \varepsilon - \mu}{kT}} + 1}$$

ε_s is a bottom of s-band

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

$\varepsilon_1, \varepsilon_2$ are the bottom and top of d-band

$\mu(T)$ is a chemical potential



$$m = \frac{m_d}{m_s} \qquad \xi = \frac{m+1}{2}$$

$$q_M = \frac{mp}{\xi}, \quad q_N = \frac{p_d + mp}{1+\xi}, \quad q_A = \frac{p_d - mp}{1+\xi}$$

$$0 \le p \le \frac{\xi p_d}{m(1+2\xi)}$$

$$\int_0^{q_M} dq \int_{mp-\xi q}^{mp+\xi q} dp' + \int_{q_M}^{q_A} dq \int_{-mp+\xi q}^{p_d} dp' + \int_{q_A}^{q_N} dq \int_{-mp+\xi q}^{p_d - q} dp'$$

Average s-d electron collision frequency

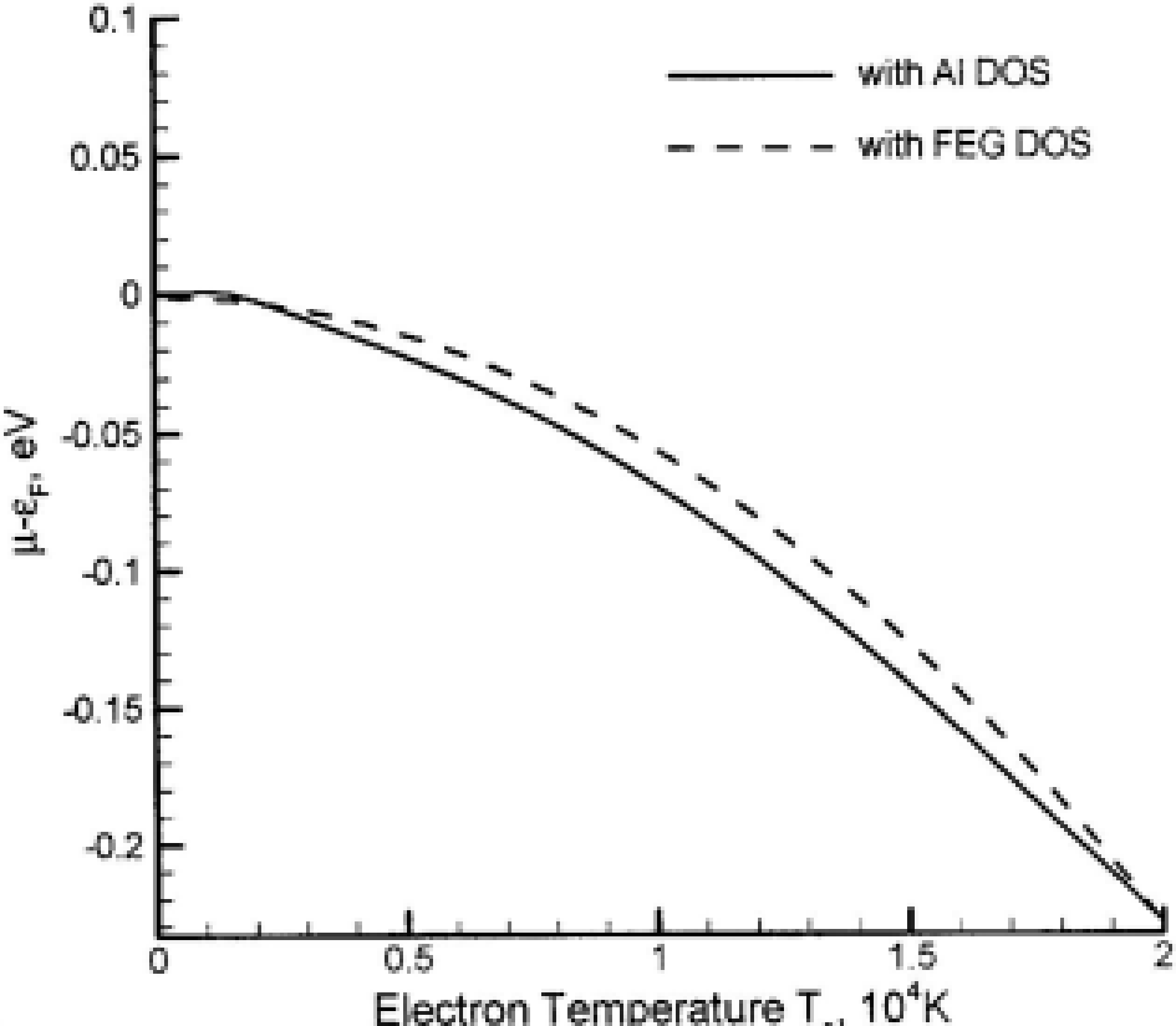
When having the frequency of collisions of the s-electron with given momentum *p* we can obtain the thermal conductivity coefficient due to s-d electron scattering:

$$\kappa_{sd}(T) = \frac{k}{3}\int(\varepsilon-\mu)\left(-\frac{\partial f_s}{\partial\varepsilon}(\varepsilon)\right)\left(\frac{\partial\mu}{\partial T}+\frac{\varepsilon-\mu}{T}\right)\frac{\mathrm{v}_s^2(p)}{\nu(p)}\frac{p^2dp}{\pi^2\hbar^3}$$

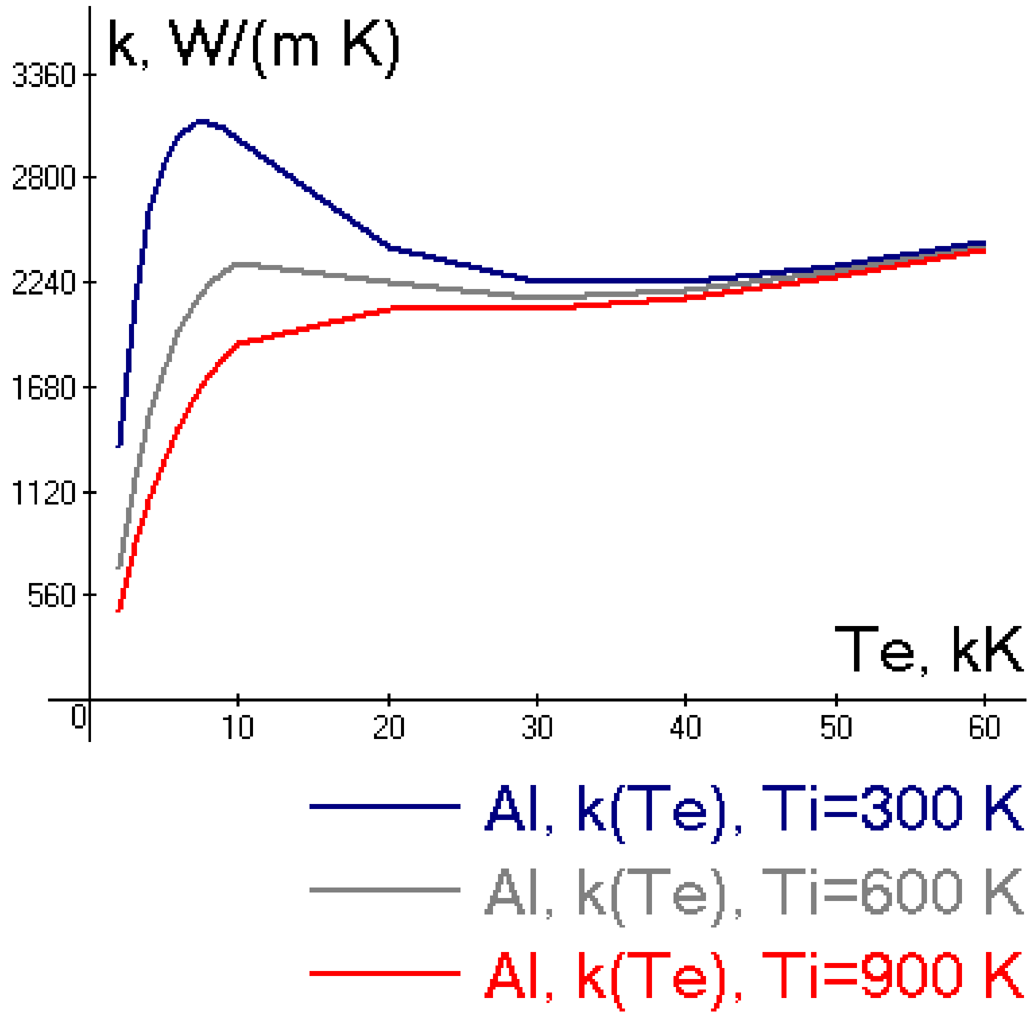
Then we define the average s-d collision frequency by using its Drude relation with thermal conductivity coefficient , mean squared velocity of s-electrons and their heat capacity per unit volume

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

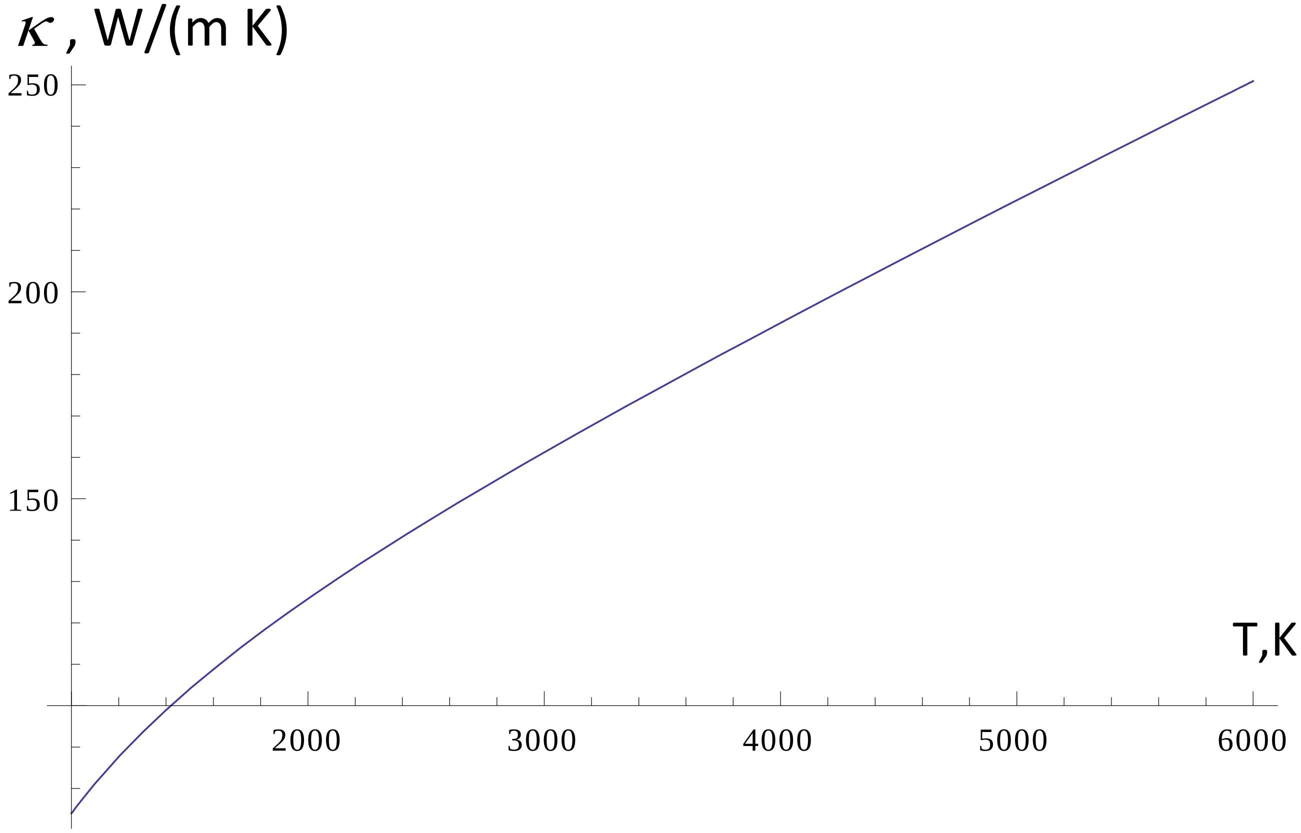
Chemical potential of Al



Коэффициент теплопроводности алюминия

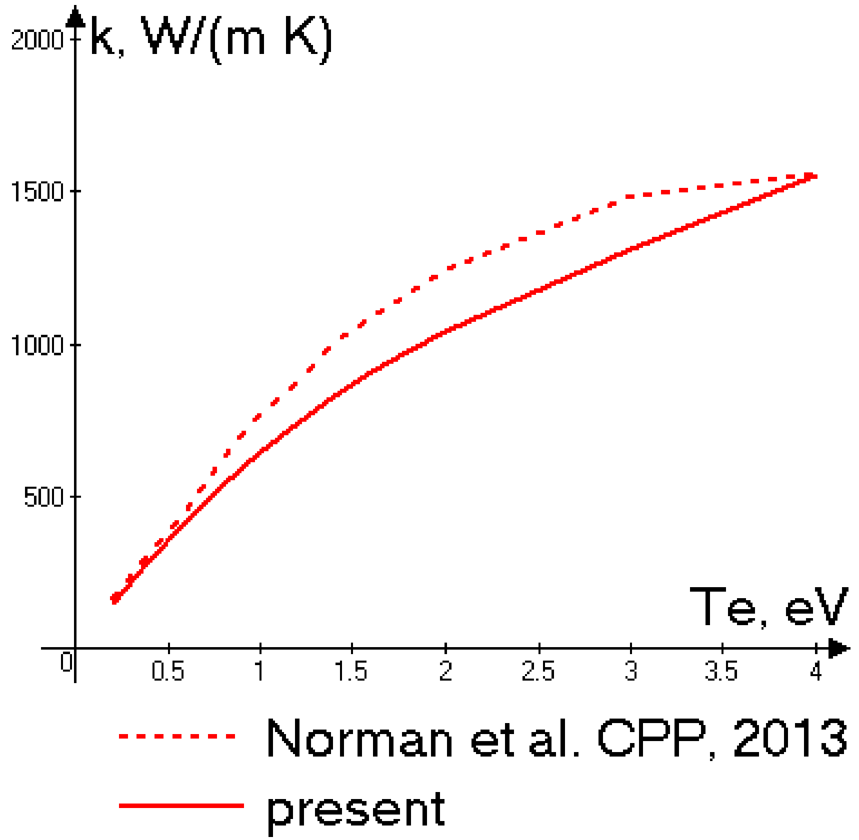


Квантовое молекулярно-динамическое моделирование теплопроводности алюминия в равновесном (Te=Ti=T) случае



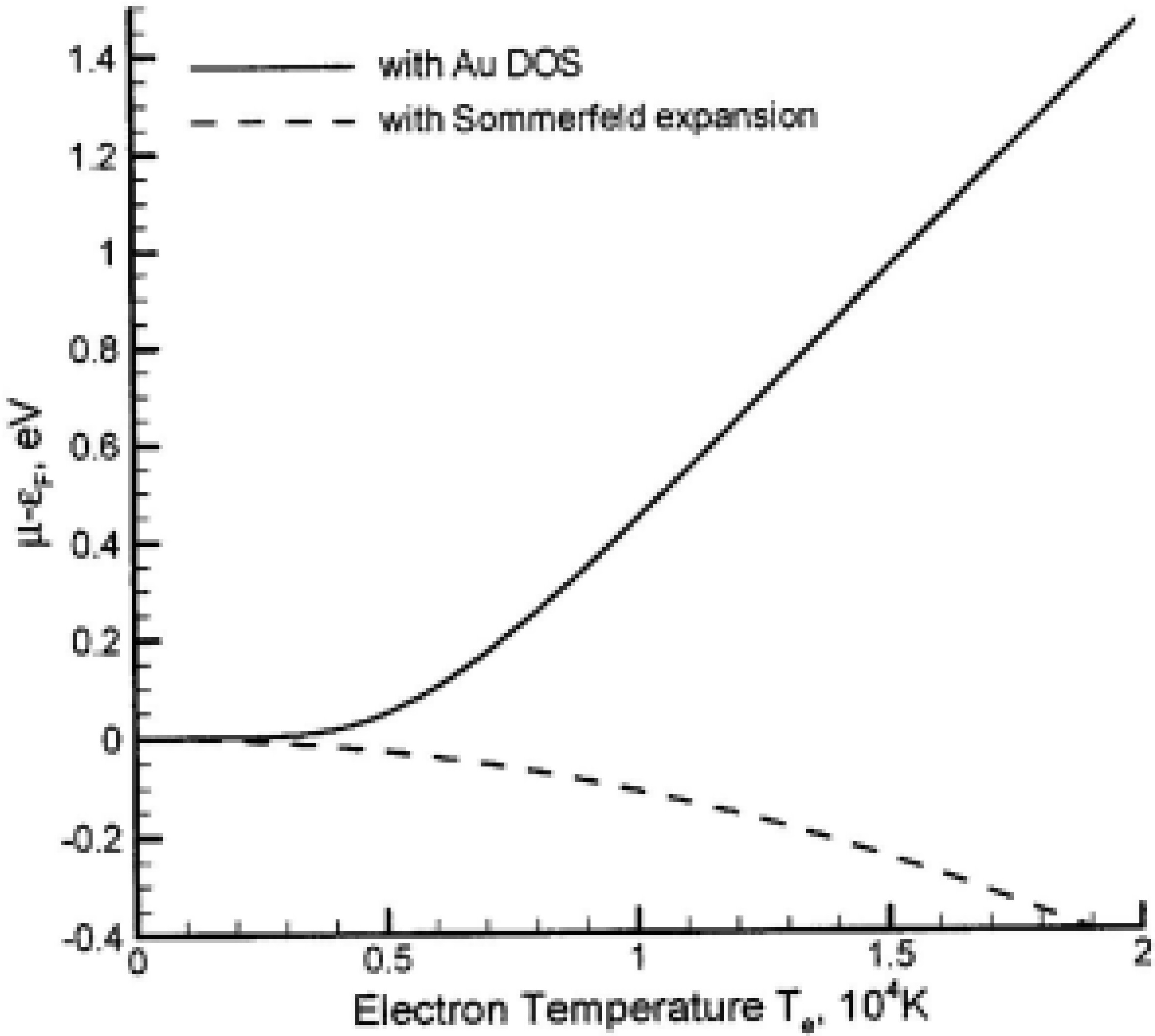
V. Recoules and J. Crocombette, Phys.Rev. B72, 104202 (2005).

Сравнение с расчетами по квантовой молекулярной динамике, алюминий, Ti=2000 K, плотность 2.35 g/cc

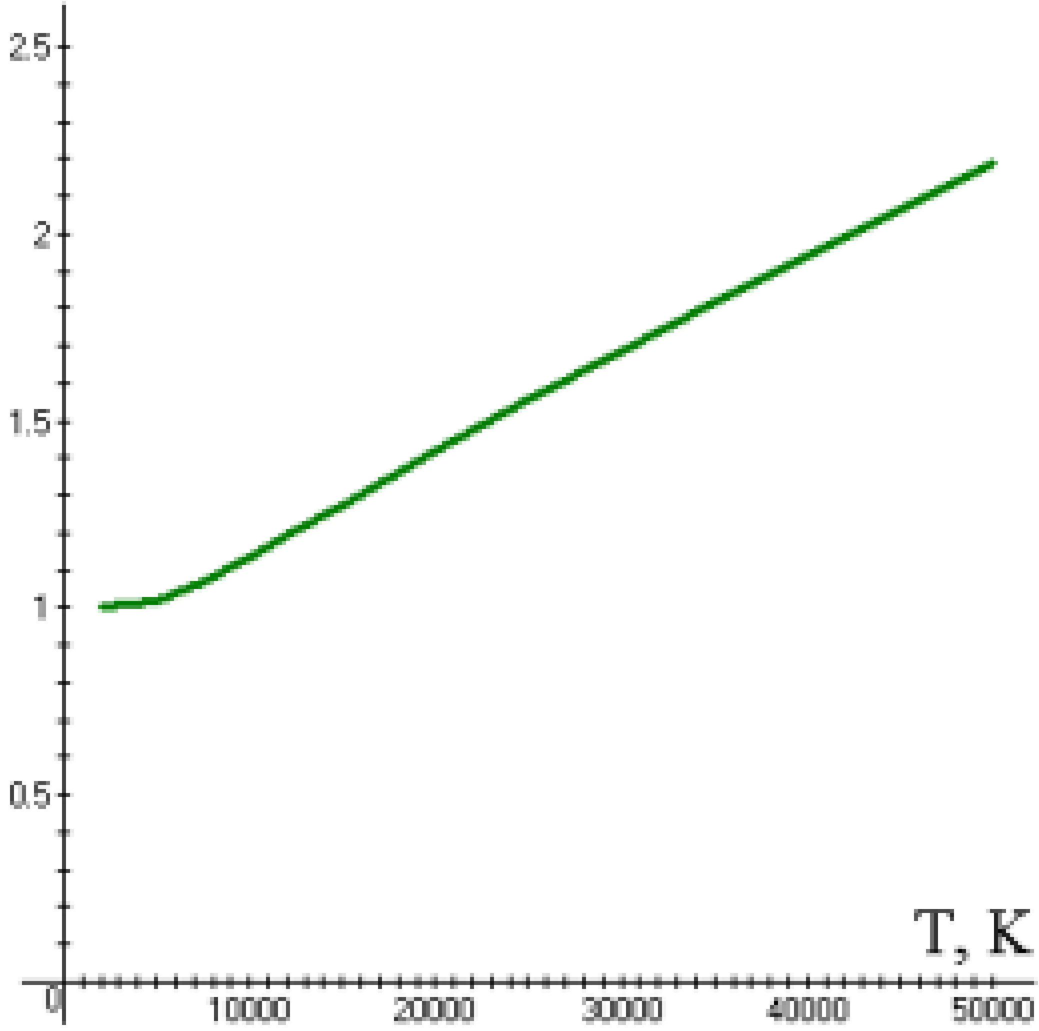


$$\kappa_{si}(T_e, T_i) = \kappa_R(T_i)\cdot \frac{\dfrac{2m_s}{3\pi^2}\displaystyle\int\left(\frac{\varepsilon_s+\varepsilon-\mu}{T_e}+\frac{\partial\mu}{\partial(T_e)}\right)(\varepsilon_s+\varepsilon-\mu)\varepsilon d\varepsilon}{\dfrac{2}{9}m_s\mu_0 T_i\left[1-\dfrac{1}{4}\pi^2\left(\dfrac{T_i}{-\varepsilon_s}\right)^2\right]}$$

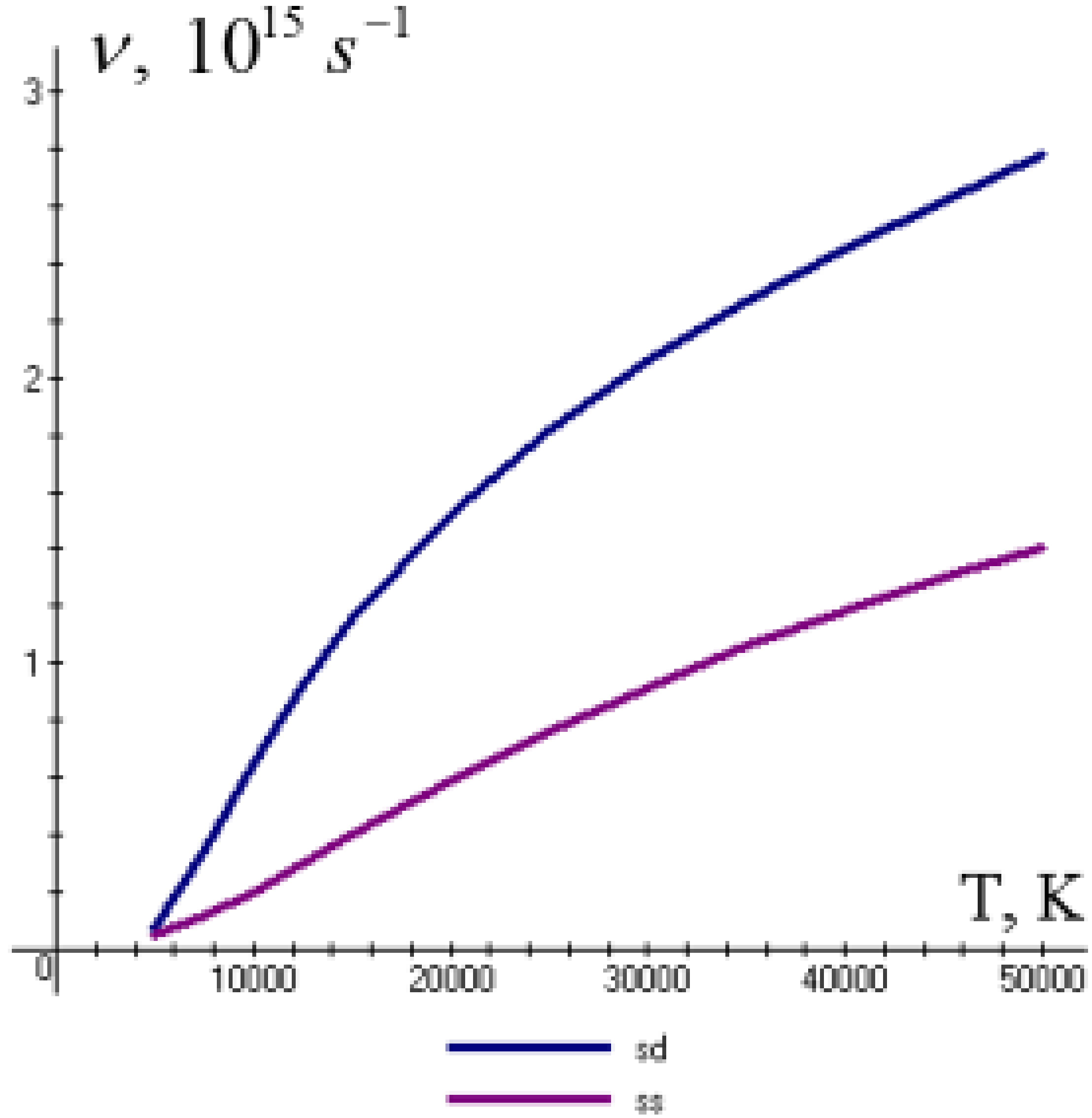
Chemical potential of Au



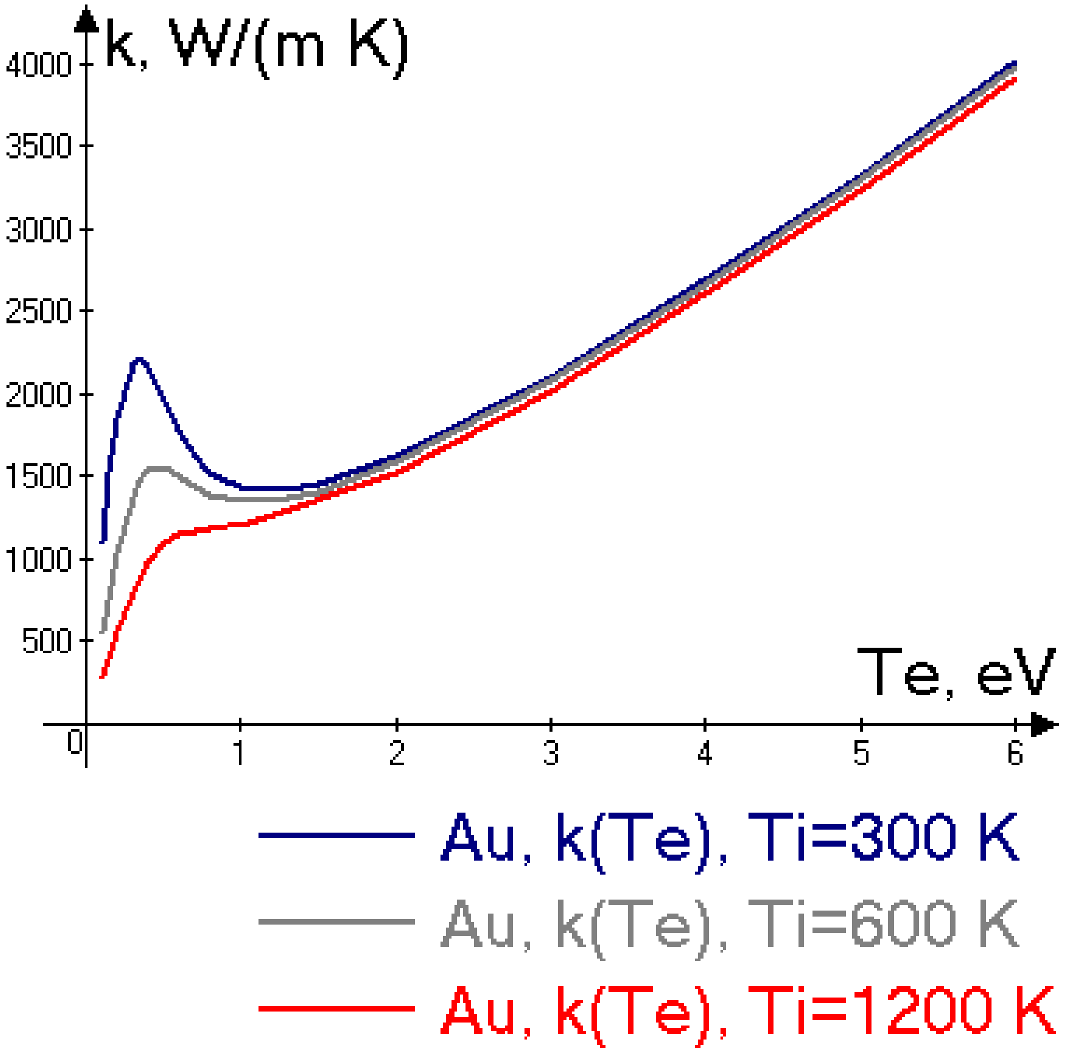
Au. Number of s-electrons per atom



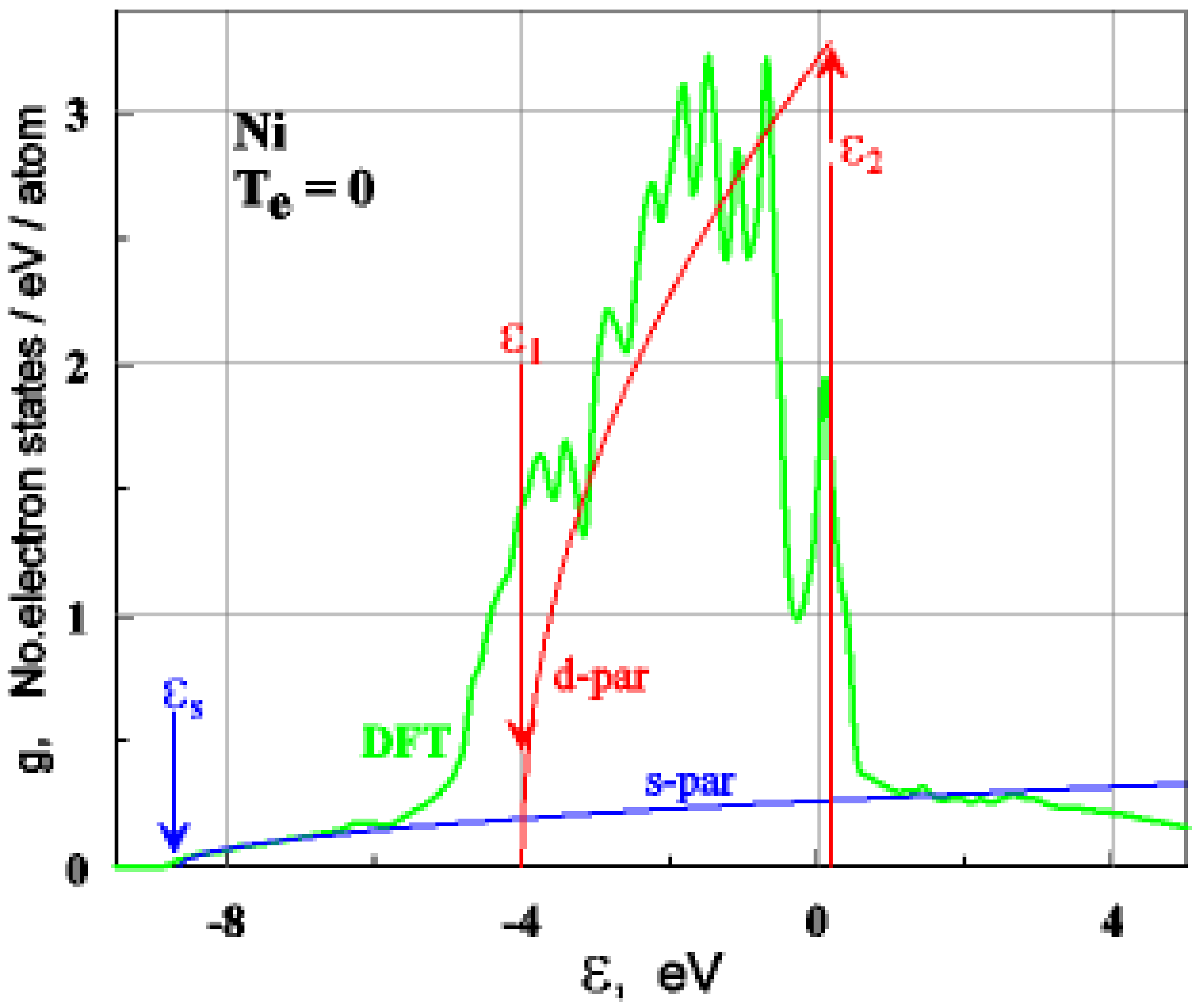
Au electron-electron collision frequency



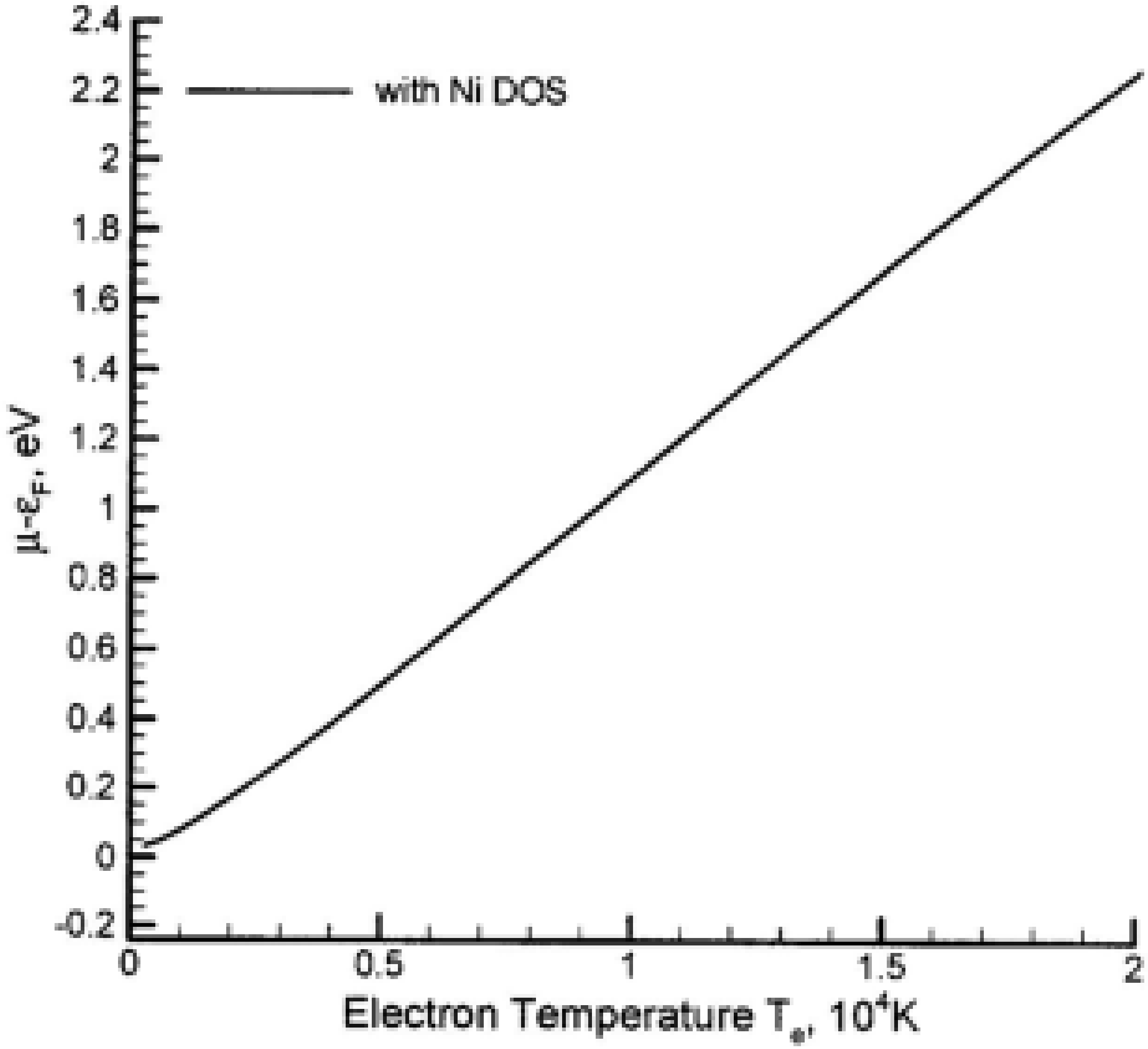
Коэффициент теплопроводности золота как функция электронной температуры



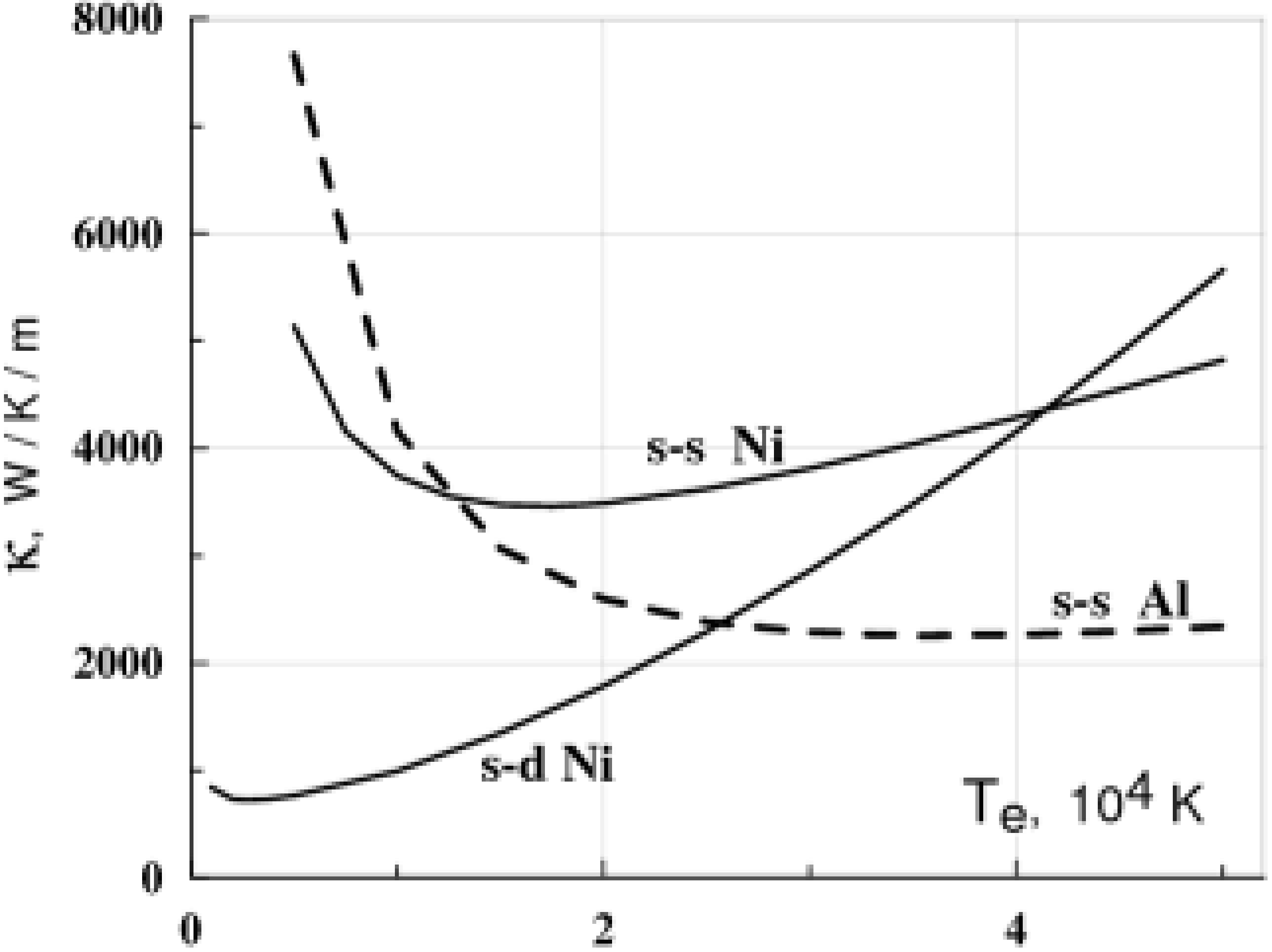
Nickel electron density of states and its parabolic approximation



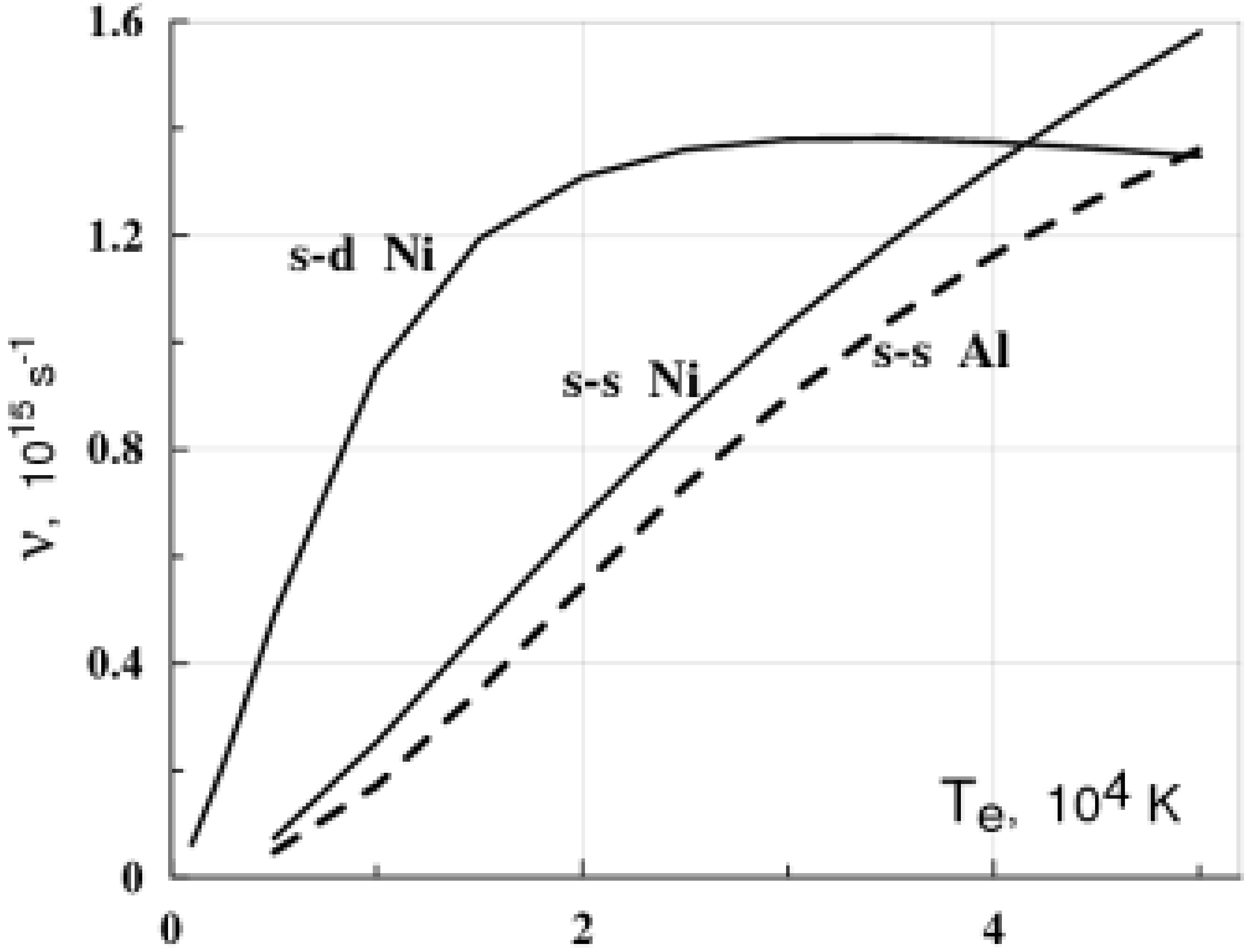
Chemical potential of Ni



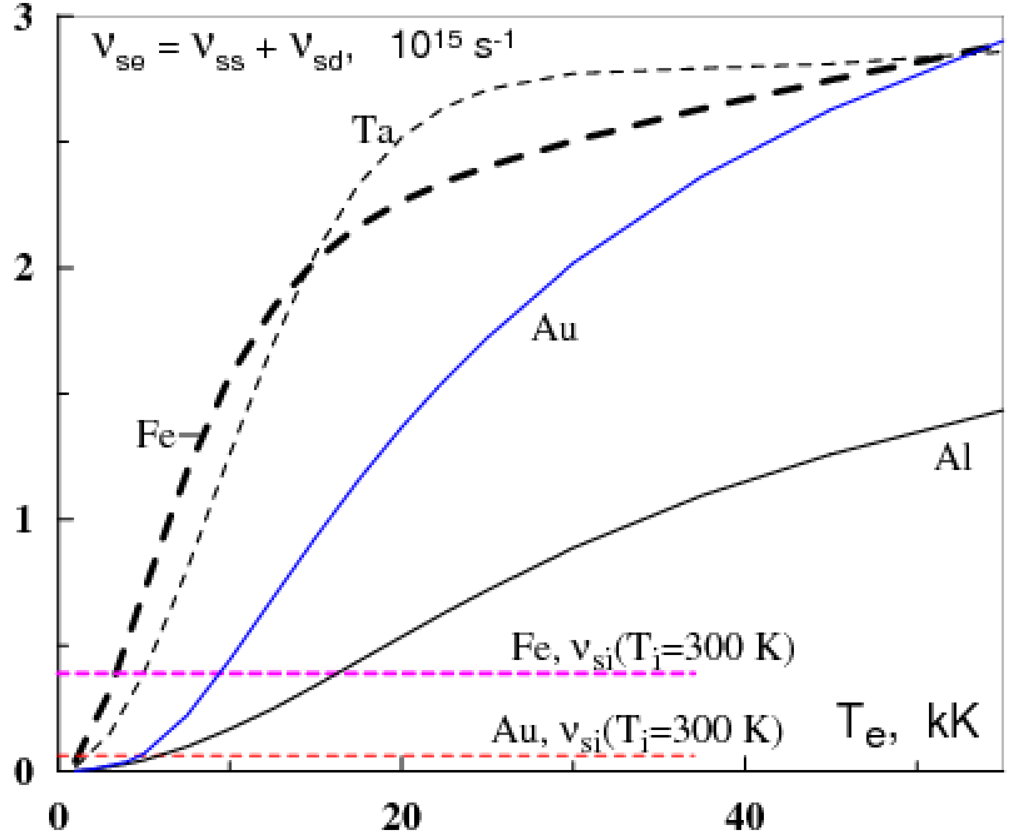
Thermal conductivity coefficient of Ni and Al due to electron-electron scattering



Average frequency of electron-electron collisions in Ni and Al as a function of electron temperature



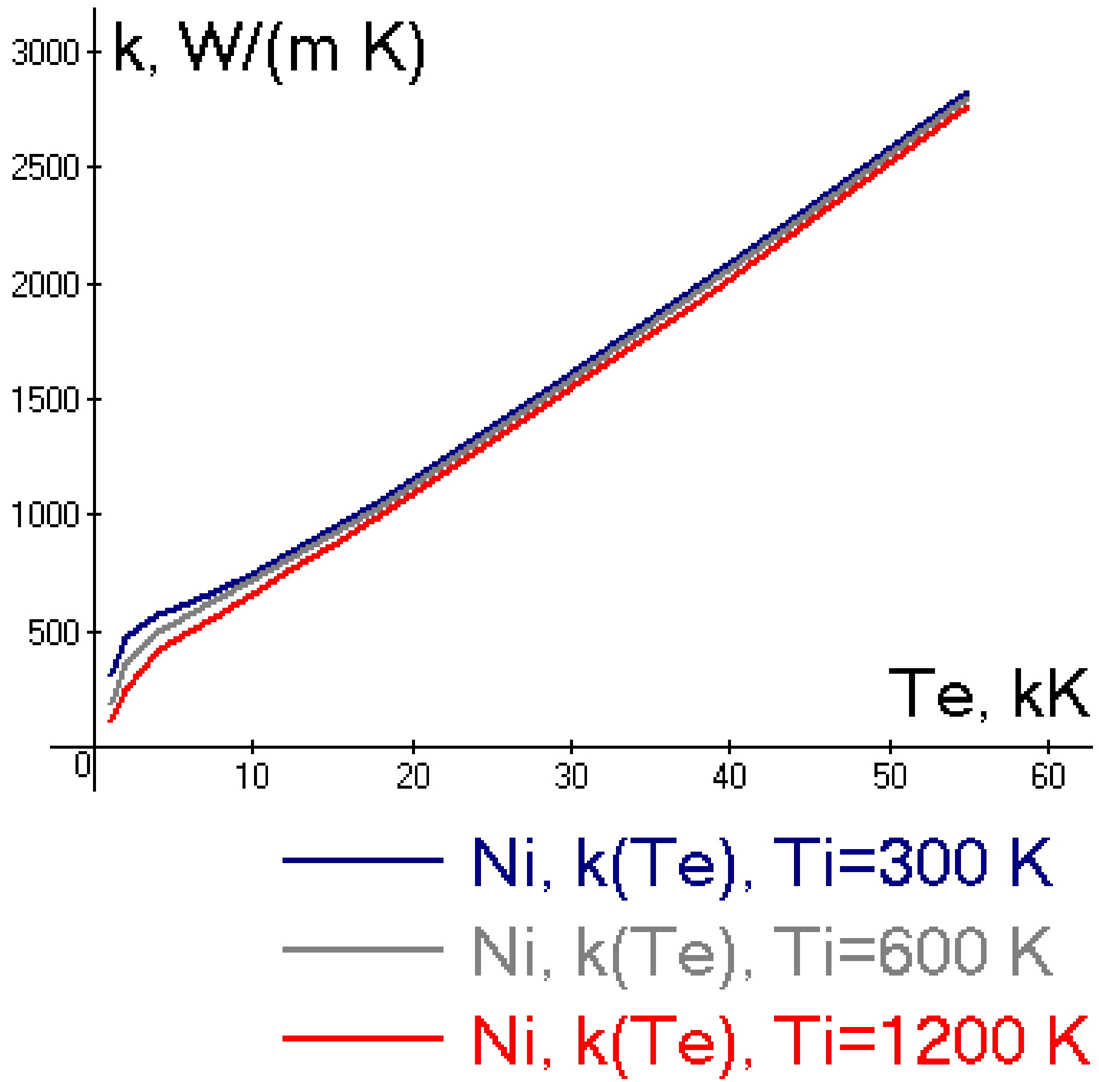
Эффективная частота электрон-электронных столкновений в зависимости от электронной температуры



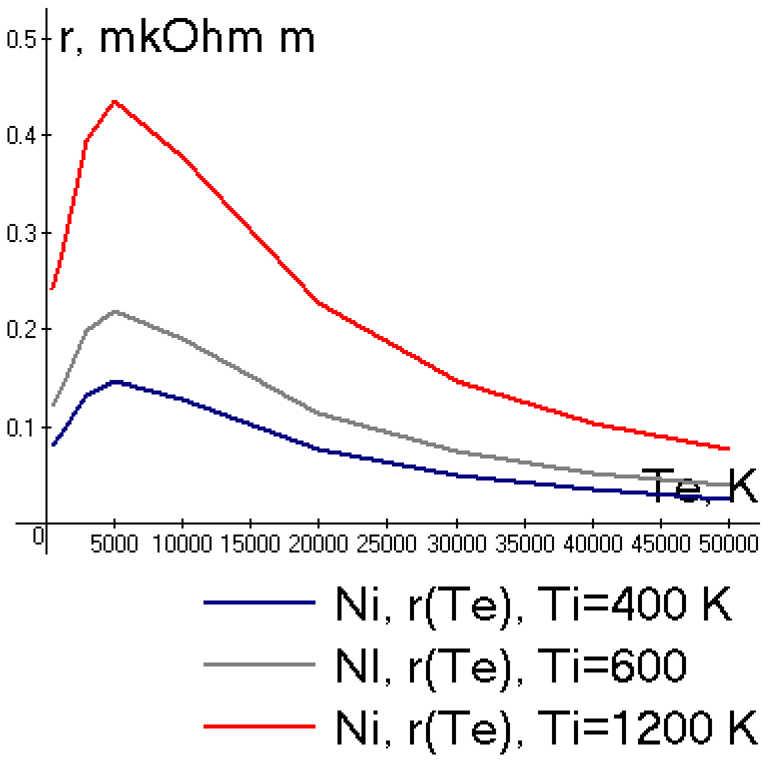
$$\kappa = \frac{1}{3}\int\left(\frac{\varepsilon-\mu}{T_e}+\frac{\partial\mu}{\partial T_e}\right)(\varepsilon-\mu)\frac{\mathrm{v}^2}{\nu(p)}\frac{p^2dp}{\pi^2\hbar^3}$$

$$\nu_{eff} = \frac{C_V\overline{\mathrm{v}}^2}{3\kappa}$$

Коэффициент теплопроводности никеля в зависимости от электронной температуры Te



Удельное сопротивление никеля в зависимости от температуры электронов



Within the effective mass approximation

$$\varepsilon = \frac{p^2}{2m_s}\,, \quad \varepsilon' = \frac{p'^2}{2m_d} \qquad \begin{aligned} m_s &= 1.1m \\ m_d &= 6.8m \end{aligned}$$

(никель)

Energy conservation

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

In terms of variables α and β

$$\Phi(\alpha,\beta) = f_d(\varepsilon')\left[1 - f_s(\varepsilon-\alpha)\right]\left[1 - f_d(\varepsilon'+\beta)\right] + f_s(\varepsilon-\alpha) f_d(\varepsilon'+\beta)\left[1 - f_d(\varepsilon')\right]$$

In terms of variables α and β the collision frequency of s-electrons having the momentum $\mathbf{p}$ with d-electrons takes a form

$$\nu(\mathbf{p}) = \nu(p) = \frac{2\pi}{\hbar}\int\left(\frac{4\pi e^2}{q^2/\hbar^2+\kappa^2}\right)^2\frac{d^3q}{(2\pi\hbar)^3}\int\frac{d^3p'}{(2\pi\hbar)^3}\Phi(\alpha,\beta)\delta(\alpha-\beta)$$

Frequency of sd-sd collisions as a two-dimensional integral in $p' - q$ plane

At given $\mathbf{p}$ introduce polar and azimuthal angles of vector $\mathbf{q}$ θ and φ (θ Is the angle between $\mathbf{p}$ and $\mathbf{q}$) and the variable $t = -\cos\theta$

At given $\mathbf{q}$ introduce polar and azimuthal angles of vector $\mathbf{p}'$ θ' and φ' and the variable $t' = -\cos\theta'$

Then

$$\alpha = \frac{2pqt - q^2}{2m_s}, \qquad d^3q = \frac{2\pi m_s q}{p} dq d\alpha$$

$$\beta = \frac{2p'qt' + q^2}{2m_d}, \qquad d^3p' = \frac{2\pi m_d p'}{q} dp' d\beta$$

$$\nu(p) = \frac{2\pi}{\hbar} \int \left(\frac{4\pi e^2}{q^2/\hbar^2 + \kappa^2} \right)^2 \frac{dq}{(2\pi\hbar)^3} \times$$

$$\int \frac{2p'dp'}{(2\pi\hbar)^3} \frac{2\pi m_s}{p} 2\pi m_d \Phi(\alpha, \beta) \delta(\alpha - \beta) d\alpha d\beta$$

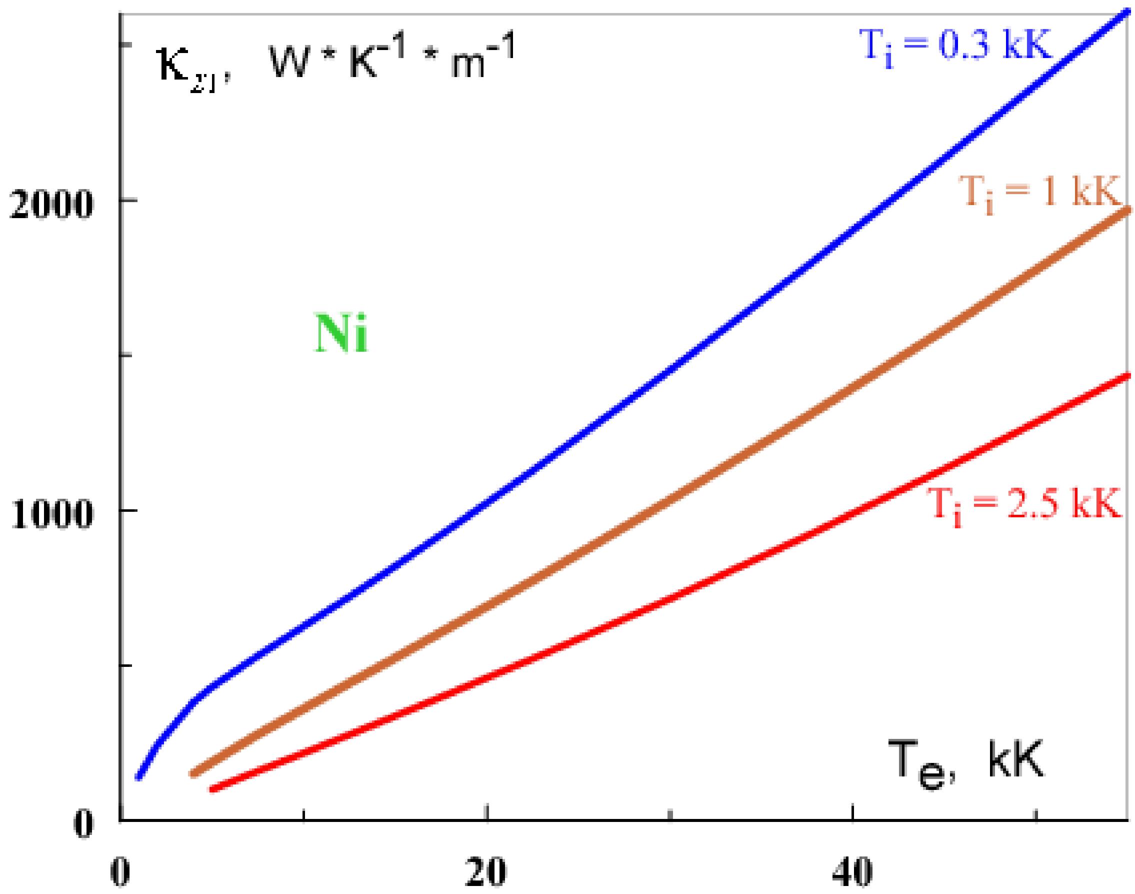
After integration over β because of the presence of δ -function

$$\nu(p) = \frac{2\pi}{\hbar} \int \left(\frac{4\pi e^2}{q^2/\hbar^2 + \kappa^2} \right)^2 \frac{dq}{(2\pi\hbar)^3} \int \frac{2p'dp'}{(2\pi\hbar)^3} \frac{2\pi m_s}{p} 2\pi m_d \Phi(\alpha, \alpha) d\alpha$$

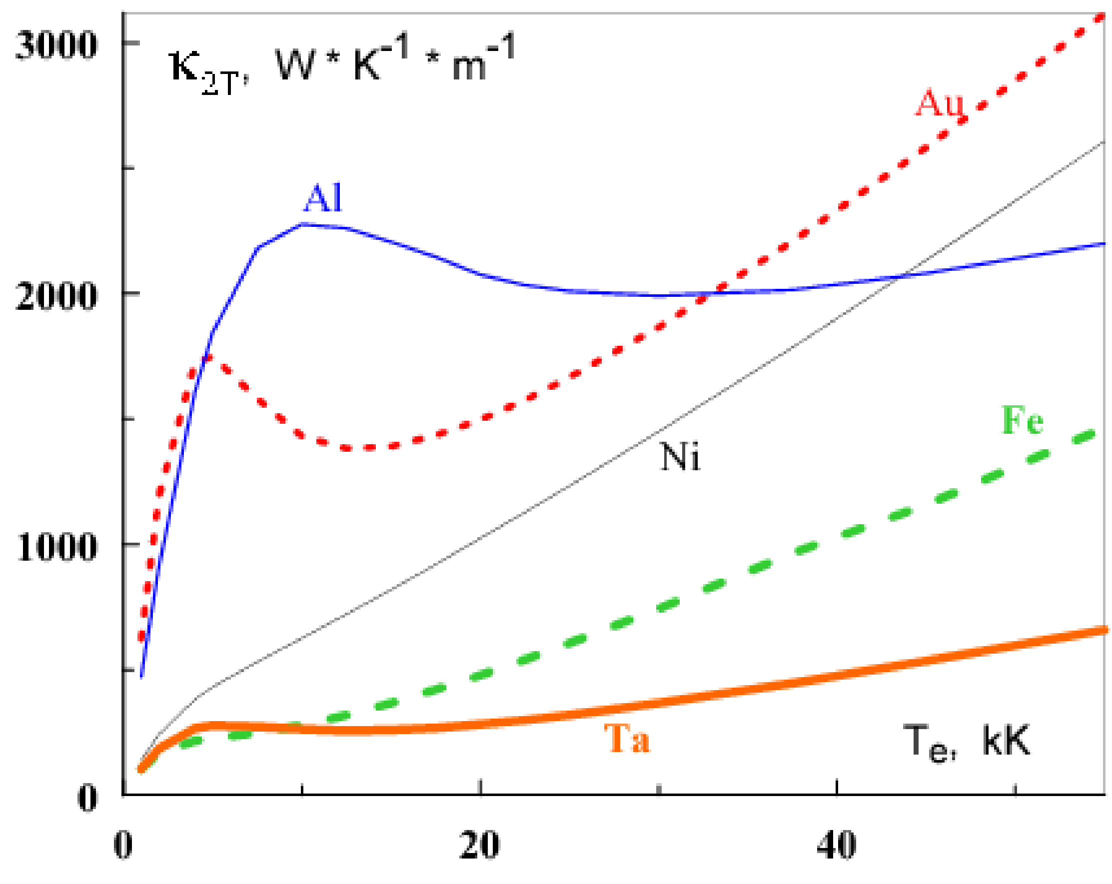
Because of dependence $\alpha'(p,p',q)$ and $\alpha''(p,p',q)$ we obtain

$$\nu(p) = \frac{2\pi}{\hbar}\int\left(\frac{4\pi e^2}{q^2/\hbar^2+\kappa^2}\right)^2 \frac{dq}{(2\pi\hbar)^3}\int\frac{2p'}{(2\pi\hbar)^3}\frac{2\pi m_s}{p}2\pi m_d$$
$$\times\widetilde{\Phi}(\alpha'(p,p',q),\alpha''(p,p',q))dp'$$

For given ***p*** the frequency of collisions is a two-dimensional integral in $p'-q$ plane

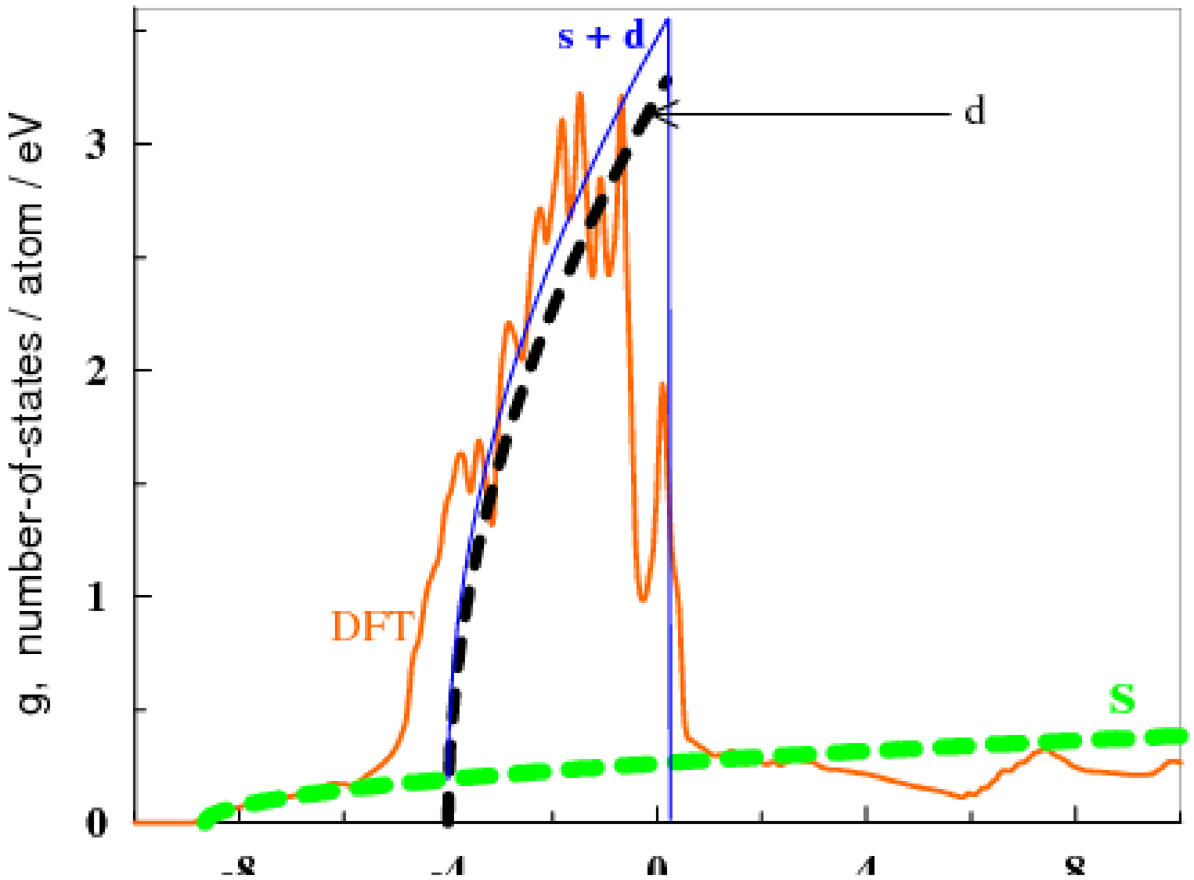


Kэл, W * K-1 * m-1
Ti = 0.3 kK
Ti = 1 kK
Ti = 2.5 kK
Ni
Te, kK
2000
1000
0
0
20
40

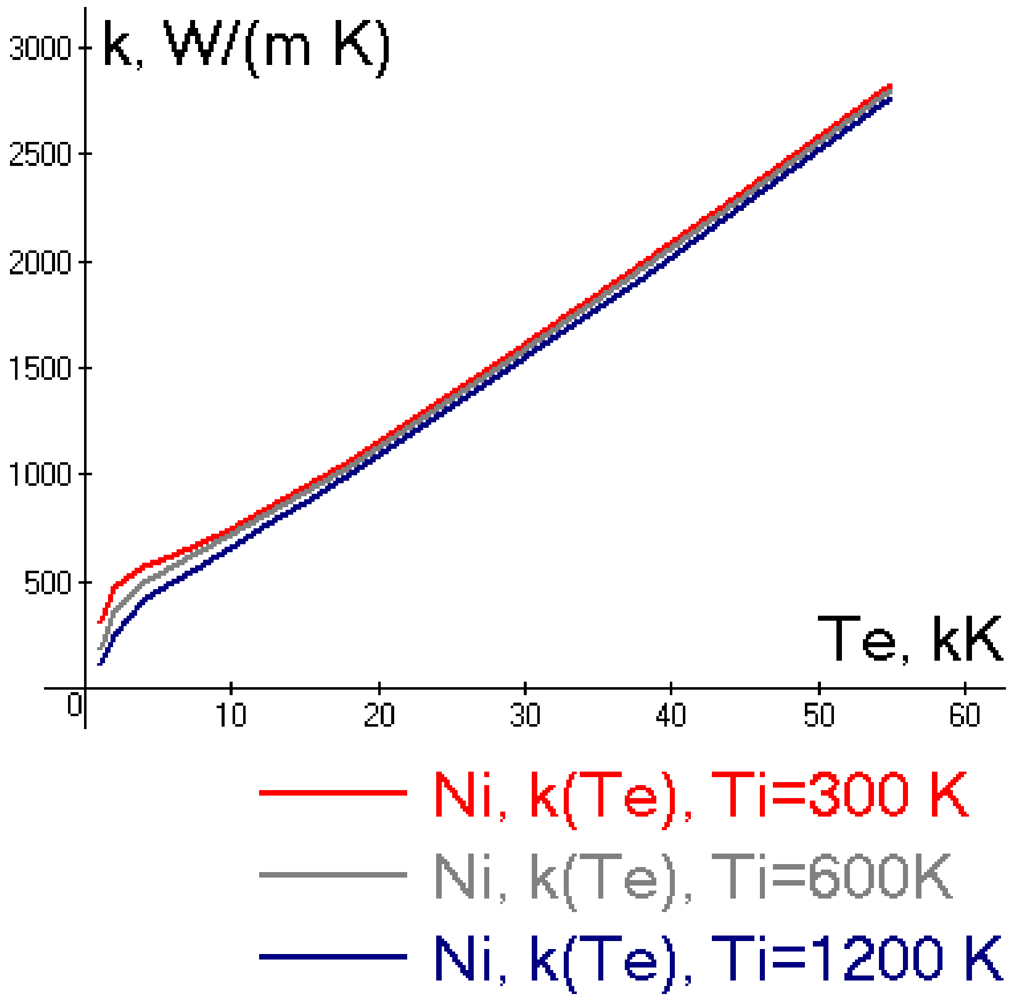


κ2T, W * K-1 * m-1
Au
Al
Fe
Ni
Ta
Te, kK
3000
2000
1000
0
0
20
40

Плотность состояний никеля



Коэффициент теплопроводности никеля в зависимости от электронной температуры Te



$$\kappa_{si}(T_e, T_i) = \kappa_R(T_i) \cdot \frac{\dfrac{2m_s}{3\pi^2} \displaystyle\int \left(\frac{\varepsilon_s + \varepsilon - \mu}{T_e} + \frac{\partial \mu}{\partial (T_e)} \right) (\varepsilon_s + \varepsilon - \mu) \varepsilon d\varepsilon}{\dfrac{2}{9} m_s \mu_0 k T_i \left[1 - \dfrac{1}{4} \pi^2 \left(\dfrac{T_i}{-\varepsilon_s} \right)^2 \right]}$$