

TWO-TEMPERATURE MICROSCALE HEAT TRANSFER MODEL. PART I: DETERMINATION OF ELECTRONS PARAMETERS

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Abstract. Two-temperature microscale heat transfer model is presented. This model contains two energy equations determining the heat exchange in the electron gas and the metal lattice. A key issue in the application of this model is the proper description of temperature dependent thermophysical parameters of the material considered and this problem is discussed here. In this part the determination of electrons thermophysical parameters is presented.

Introduction

Micro-scale heat transfer in the metals can be described in different ways [1-5]. In this paper the microscopic, two-temperature model presented among others in [1, 2, 6] is presented. This model involves two energy equations determining the heat exchange in the electron gas and the metal lattice. So, the equations creating the model discussed can be written in the form

$$C_e(T_e) \frac{\partial T_e}{\partial t} = \nabla [\lambda_e(T_e, T_l) \nabla T_e] - G(T_e) (T_e - T_l) + Q(x, t) \quad (1)$$

and

$$C_l(T_l) \frac{\partial T_l}{\partial t} = \nabla [\lambda_l(T_l) \nabla T_l] - G(T_l) (T_e - T_l) \quad (2)$$

where $T_e = T_e(x, t)$, $T_l = T_l(x, t)$ are the temperatures of electrons and lattice, respectively, $C_e(T_e)$, $C_l(T_l)$ are the volumetric specific heats, $\lambda_e(T_e, T_l)$, $\lambda_l(T_l)$ are the thermal conductivities, $G(T_e)$ is the coupling factor which characterizes the energy exchange between phonon and electrons [6], $Q(x, t)$ is the source term.

This model describes, among others, the thermal processes proceeding in metals subjected to the laser pulse or high-energy ion bombardment of metal targets [6].

A key issue in the application of two-temperature model is the proper description of temperature dependent thermophysical properties of the material and this problem is discussed here. In this part of the paper the models assuring determination of electrons thermophysical parameters are shown.

1. Electrons heat capacity

In order to define the electron heat capacity $C_e(T_e)$, at first the internal total electron energy is calculated [5-7]

$$U_e = \int_0^{\infty} f(E, \mu, T_e) g(E) E dE \quad (3)$$

where $g(E)$ is the electron density of states (DOS) at the energy level E and $f(E, \mu, T_e)$ is the Fermi distribution function.

The Fermi distribution function is defined as

$$f(E, \mu, T_e) = \frac{1}{\exp\left(\frac{E - \mu}{k_B T_e}\right) + 1} \quad (4)$$

where $\mu = \mu(T_e)$ [eV] is the chemical potential at the temperature T_e [K] and k_B is the Boltzmann constant ($k_B = 1.381 \cdot 10^{-23}$ J/K).

At the absolute temperature $T_e = 0$ K, $f(E, \mu, T_e) = 1$ when $E < \mu$, and $f(E, \mu, T_e) = 0$ when $E > \mu$. It should be pointed out that $\mu(0) = \mu_F = E_F$ is called the Fermi energy.

The Fermi energy can be calculated using the formula [7]

$$E_F = \frac{\hbar^2}{2m_e} \left(3\pi^2 n_e\right)^{\frac{2}{3}} \quad (5)$$

where $\hbar = h/(2\pi)$, h is the Planck constant ($h = 6.6260693 \cdot 10^{-34}$ J·s = $4.135667443 \cdot 10^{-15}$ eV·s), m_e is the electron mass ($m_e = 9.109 \cdot 10^{-31}$ kg) and n_e is the number of electrons N_e per unit of volume V ($n_e = N_e/V$).

Additionally, the Fermi temperature T_F is defined

$$T_F = \frac{T_e}{k_B} \quad (6)$$

and the Fermi velocity v_F is introduced. The velocity v_F can be determined from the formula [7]

$$v_F = \frac{\hbar}{m_e} \left(3 \pi^2 n_e \right)^{\frac{1}{3}} \quad (7)$$

In the Table 1 the Fermi parameters of selected metals are collected, while Figure 1 illustrates the distribution of Fermi function (4) for temperatures $T_e = 0, T_e = 0.1T_F, T_e = 0.25T_F$ and Fermi energy $\mu = E_F$ for selected metals.

Table 1

Fermi parameters of selected metals

Metal	Electron number density $n_e [10^{28}/\text{m}^3]$	Fermi energy $E_F [\text{eV}]$	Fermi temperature $T_F [10^4 \text{ K}]$	Fermi velocity $v_F [10^6 \text{ m/s}]$
Li	4.70	4.75	5.51	1.29
Na	2.65	3.24	3.77	1.07
K	1.40	2.12	2.46	0.86
Cu	8.45	7.03	8.16	1.57
Ag	5.85	5.50	6.38	1.39
Au	5.90	5.53	6.41	1.40
Mg	8.60	7.11	8.24	1.58
Ca	4.60	4.68	5.43	1.28
Zn	13.10	9.41	10.91	1.82
Fe	17.00	11.20	13.00	1.98
Al	18.10	11.70	13.54	2.03
Sn	14.80	10.20	11.84	1.90
Pb	13.20	9.45	10.97	1.82
W	5.91	5.55	6.42	1.39
Ti	13.80	9.74	11.30	1.85

The electron density of states $g(E)$ appearing in equation (3) can be obtained using FEG model (free electron gas model) [4] and then

$$g(E) = 4 \pi \left(\frac{2 m_e}{h^2} \right)^{\frac{3}{2}} \sqrt{E} \quad (24)$$

In the newest publications [6, 8] the electron density of states can be determined from the electronic structure calculations performed within the density functional theory.

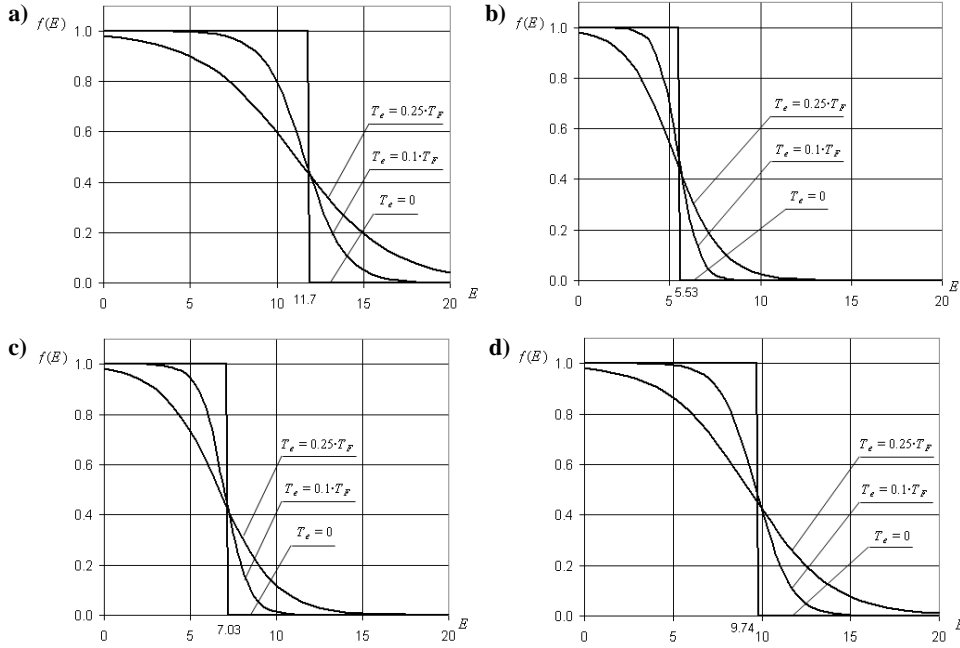


Fig. 1. Fermi function: a) Al, b) Au, c) Cu, d) Ti

The number of electrons $N_e(E)dE$ of energy between E and $E + dE$ in the unit of volume at the temperature T_e is equal to the product of density of states and Fermi distribution function (4)

$$N_e(E) dE = g(E) f(E, \mu, T_e) dE \quad (8)$$

This function shown in Figure 2 (for electron density of states described by equation (8)) is called the distribution function of free electrons.

The total number of electrons is equal to

$$N_e = \int_0^{\infty} g(E) f(E, \mu, T_e) dE \quad (9)$$

The electron heat capacity can be calculated as the derivative of the total electron energy (3) with respect to the electron temperature

$$C_e(T_e) = \frac{\partial U_e}{\partial T_e} = \int_0^{\infty} \frac{\partial f(E, \mu(T_e), T_e)}{\partial T_e} g(E) E dE \quad (10)$$

Determination of $C_e(T_e)$ is not easy because the evaluation of $\partial f/\partial T_e$ requires the knowledge of a chemical potential as a function of electrons temperature $\mu(T_e)$.

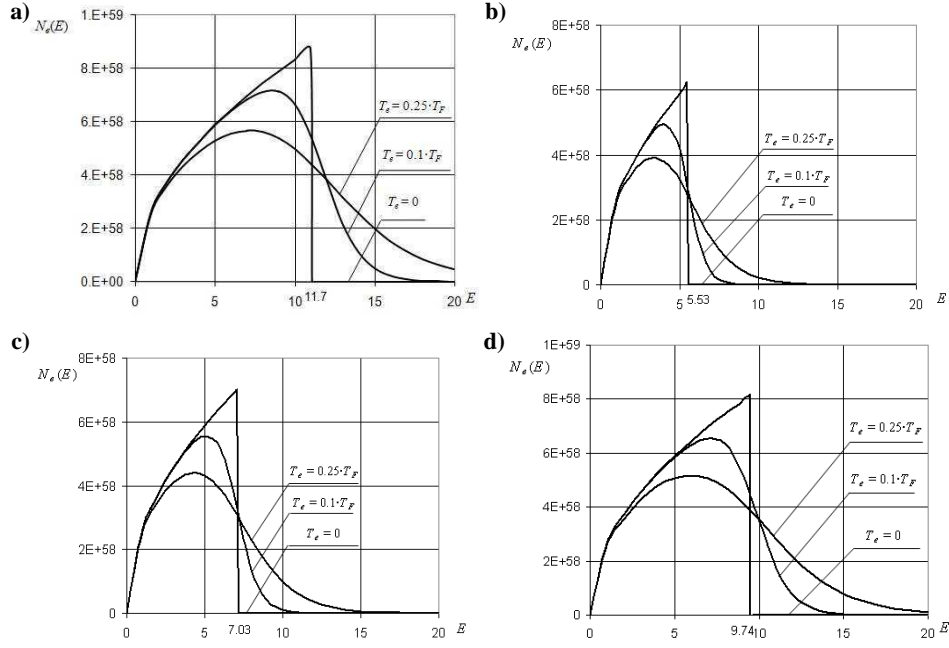


Fig. 2. Distribution function of free electrons $N_e(E)$: a) Al, b) Au, c) Cu, d) Ti

At the low electron temperatures the Sommerfeld expansion is commonly used [7]. As is known, at the temperature $T_e = 0$ ($T_e \rightarrow 0$), the Fermi function (4) $f(E, \mu_F, T_e) = 1$ when $E < \mu_F$, and $f(E, \mu_F, T_e) = 0$ when $E > \mu_F$. So (c.f. equation (10))

$$N_e = \int_0^{\infty} f(E, \mu, 0) g(E) dE = \int_0^{\mu_F} g(E) dE \quad (10)$$

At the low temperature T_e the Fermi function is constant (0 or 1) except the narrow interval $[\mu_F - \mu, \mu_F + \mu]$ as shown in Figure 3. In this case the following approximation can be taken into account

$$N_e = \int_0^{\mu} f(E, \mu, T_e) g(E) dE = \int_0^{\mu_F} g(E) dE + (\mu - \mu_F) g(\mu_F) \quad (11)$$

Sommerfeld proposed the following approximation [7]

$$N_e = \int_0^{\infty} f(E, \mu, T_e) g(E) dE = \int_0^{\mu} f(E, \mu, T_e) g(E) dE + \frac{\pi^2 (k_B T_e)^2}{6} \frac{dg(\mu)}{d\mu} \quad (12)$$

where $g(\mu) = g(E)$ is described by equation (8).

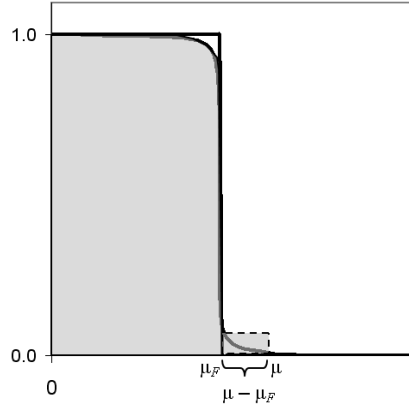


Fig. 3. Fermi function for $T_e = 0$ and for low temperature $T_e > 0$

The first component on the right-hand side of equation (14) under the assumption that $\mu \approx \mu_F$ can be substituted by formula (13), in the second component $\mu = \mu_F$ can be accepted

$$N_e = \int_0^{\mu_F} g(E) dE + (\mu - \mu_F) g(\mu_F) + \frac{\pi^2 (k_B T_e)^2}{6} g'(\mu_F) \quad (13)$$

Because the number of electrons N_e is constant and temperature independent so the first component on the right-hand side of equation (15) is equal to N_e and then

$$(\mu - \mu_F) g(\mu_F) + \frac{\pi^2 (k_B T_e)^2}{6} g'(\mu_F) = 0 \quad (14)$$

or

$$\mu = \mu_F - \frac{\pi^2 (k_B T_e)^2}{6} \frac{g'(\mu_F)}{g(\mu_F)} \quad (15)$$

From equation (8) one has

$$\frac{d g(E)}{d E} = g'(E) = \frac{1}{\pi^2} \frac{2^{\frac{1}{2}} m_e^{\frac{3}{2}}}{h^3} \frac{1}{2\sqrt{E}} \quad (16)$$

and

$$\frac{g'(E)}{g(E)} = \frac{1}{2E} \quad (17)$$

Finally

$$\mu(T_e) = \mu_F - \left[1 - \frac{1}{3} \left(\frac{\pi k_B T_e}{2\mu_F} \right)^2 \right] \quad (18)$$

To determine the electrons thermal capacity, at first the internal energy is calculated using the Sommerfeld expansion (14)

$$U_e = \int_0^{\infty} f(E, \mu, T_e) g(E) E dE = \int_0^{\mu_F} g(E) E dE + (\mu - \mu_F) g(\mu_F) \mu_F + \frac{\pi^2 (k_B T_e)^2}{6} \left. \frac{d[g(E) E]}{dE} \right|_{E=\mu_F} \quad (19)$$

and then

$$U_e = \int_0^{\infty} f(E, \mu, T_e) g(E) E dE = \int_0^{\mu_F} g(E) E dE + \mu_F (\mu - \mu_F) g(\mu_F) + \frac{\pi^2 (k_B T_e)^2}{6} \mu_F g'(\mu_F) + \frac{\pi^2 (k_B T_e)^2}{6} g(\mu_F) \quad (20)$$

On the basis of formula (16) the sum of the second and third component on the right-hand side of equation (22) is equal to zero, while the first component is temperature independent. So

$$C_e(T_e) = \frac{\partial U_e}{\partial T_e} = \frac{\pi^2 k_B^2 T_e}{3} g(\mu_F) \quad (21)$$

or

$$C_e(T_e) = \gamma T_e \quad (22)$$

where

$$\gamma = \frac{\pi^2 k_B^2 g(\mu_F)}{3} = \frac{\pi^2 k_B^2 n_e}{2 E_F} \quad (23)$$

In the case of high electron temperatures the simplification (14) is not valid and the electron heat capacity should be calculated directly from equation (11). It requires the knowledge of chemical potential as a function of electrons temperature $\mu(T_e)$. The chemical potential can be obtained from the conservation of the total number of electrons - c.f. equation (10).

In Figure 3 the course of thermal capacity described by equation (11) under the assumption that the chemical potential is calculated using the formula (10) for selected metals is shown.

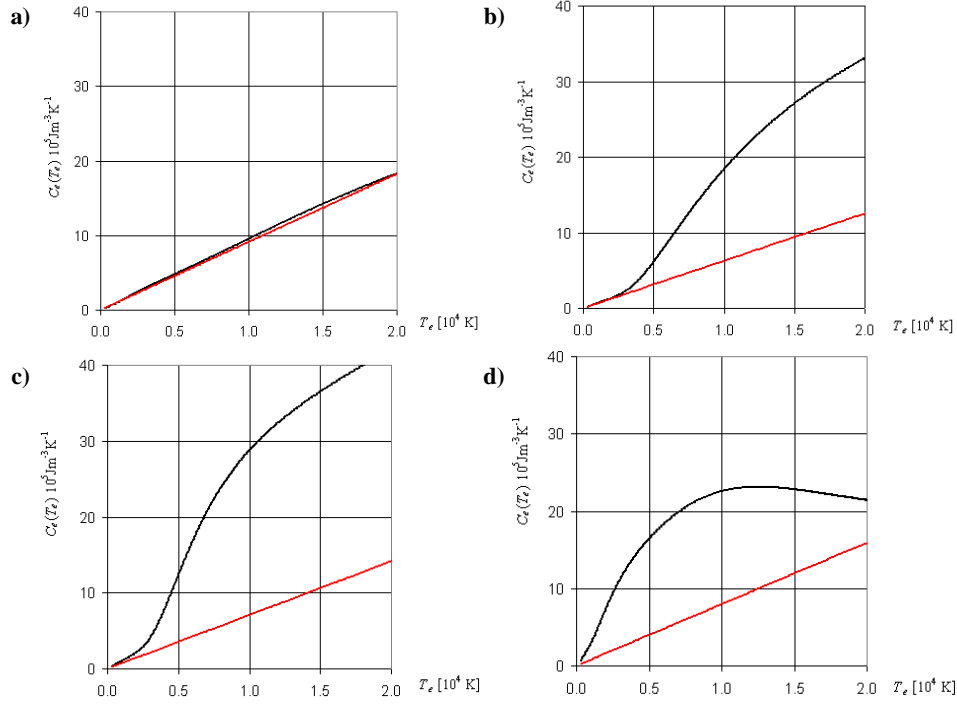


Fig. 4. Electrons thermal capacity [9]: a) Al, b) Au, c) Cu, d) Ti

2. Electrons thermal conductivity

The electrons thermal conductivity in metals is described by the Drude model relationship [7]

$$\lambda_e(T_e, T_l) = \frac{1}{3} C_e(T_e) \tau_e(T_e, T_l) v_e^2 \quad (24)$$

where $C_e(T_e)$ is the electrons thermal capacity, $\tau_e(T_e, T_l)$ is the total electron scattering time and v_e is the mean velocity of the electrons.

It is assumed that all electrons within the metal are traveling at the Fermi velocity (7), this means $v_e = v_F$.

Electrons collisions can occur with other electrons, the lattice, defects, grain boundaries and surfaces as shown in Figure 5.

Assuming that each mechanism is independent, the Matthiessen rule [7, 8] can be applied

$$\frac{1}{\tau_e} = \frac{1}{\tau_{ee}} + \frac{1}{\tau_{eph}} + \frac{1}{\tau_{ed}} + \frac{1}{\tau_{eb}} \quad (25)$$

where τ_{ee} is the electron-electron scattering time, τ_{eph} is the electron-phonon scattering time, τ_{ed} is the electron-defect scattering time and τ_{eb} is the electron-boundary scattering time.

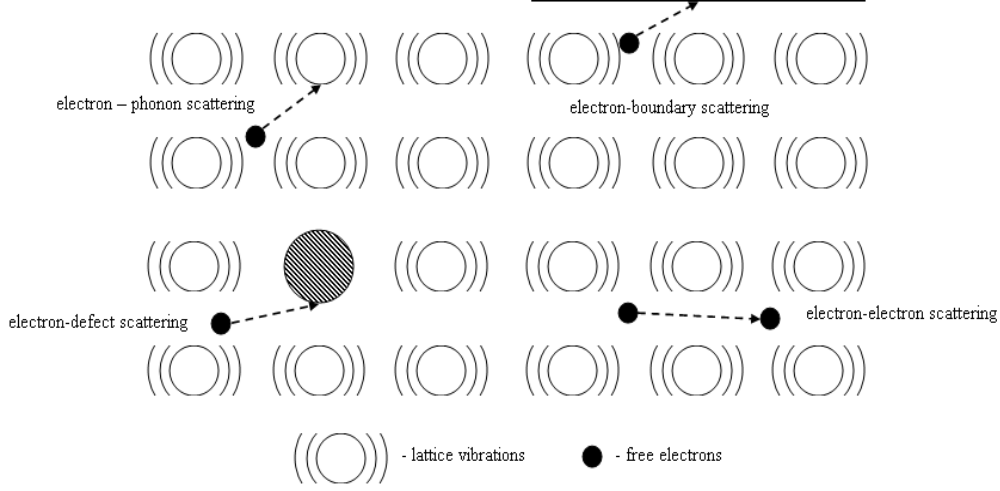


Fig. 5. Scheme of various scattering mechanisms [4]

Electron-defect and electron-boundary scattering are both typically independent of temperature, while electron-phonon scattering rate is proportional to the lattice temperature T_l , this means $1/\tau_{eph} = BT_l$ and electron-electron scattering rate is proportional to the second power of electron temperature $1/\tau_{ee} = AT_e^2$. So

$$\frac{1}{\tau_e} = \frac{1}{\tau_{ee}} + \frac{1}{\tau_{eph}} = AT_e^2 + BT_l \quad (26)$$

where A, B are typically assumed to be constant.

Taking into account the dependencies (28), (7) the electrons thermal conductivity (26) can be expressed as

$$\lambda_e(T_e, T_l) = \frac{1}{3} C_e(T_e) \frac{1}{AT_e^2 + BT_l} \frac{\hbar^2}{m_e^2} (3\pi^2 n_e)^{\frac{2}{3}} \quad (27)$$

For temperatures above the Debye temperature the electron-electron scattering in comparison with electron-phonon scattering can be neglected [7] and under the assumption that thermal capacity is described by formula (24) one has

$$\lambda_e(T_e, T_l) = \frac{\pi^2 k_B^2 n_e T_e}{3 B m_e T_l} \quad (28)$$

In numerical modelling of microscale heat transfer usually the following dependence is used [10, 11]

$$\lambda_e(T_e, T_l) = \lambda_0 \frac{T_e}{T_l} \quad (29)$$

where λ_0 is the thermal conductivity for $T_e = T_l$ at the room temperature.

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