

TWO-TEMPERATURE MICROSCALE HEAT TRANSFER MODEL. PART II: DETERMINATION OF LATTICE 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 metal lattice thermophysical parameters is presented.

Introduction

The microscopic, two-temperature model [1, 2, 3, 4, 5, 6] is as follows

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

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.

In this part of the paper the models assuring determination of lattice thermophysical parameters are shown.

1. Lattice heat capacity

The total energy of the lattice is given by equation [4, 7]

$$U_l = \int_{\omega_1}^{\omega_2} g_l(\omega) f_{BE}(\omega, T_l) h \omega d\omega \quad (3)$$

where ω_1 , ω_2 are the minimum and maximum frequency of phonons, $g_l(\omega)$ is the phonons density of states, $\hbar = h/(2\pi)$, h is the Planck constant ($h = 6.6260693 \cdot 10^{-34}$ J·s = $4.135667443 \cdot 10^{-15}$ eV·s).

The Bose-Einstein distribution function $f_{BE}(\omega, T_l)$ is defined as

$$f(\omega, T_l) = \frac{1}{\exp\left(\frac{\hbar \omega}{k_B T_l}\right) - 1} \quad (4)$$

where T_l is the lattice temperature and k_B is the Boltzmann constant ($k_B = 1.381 \cdot 10^{-23}$ J/K).

The number of phonons $N_l(\omega)d\omega$ of the frequency between ω and $\omega + d\omega$ per unit of volume is equal to the product of density of states and Bose-Einstein distribution function

$$N_l(\omega) d\omega = g_l(\omega) f_{BE}(\omega, T_l) d\omega \quad (5)$$

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

$$C_l = \frac{\partial U_l}{\partial T_l} = \int_{\omega_1}^{\omega_2} g_l(\omega) \frac{\partial f_{BE}(\omega, T_l)}{\partial T_l} \hbar \omega d\omega =$$

$$k_B \int_{\omega_1}^{\omega_2} \left(\frac{\hbar \omega}{k_B T_l}\right)^2 \frac{\exp\left(\frac{\hbar \omega}{k_B T_l}\right)}{\left[\exp\left(\frac{\hbar \omega}{k_B T_l}\right) - 1\right]^2} g_l(\omega) d\omega \quad (6)$$

They are two models for the density of states of the phonon system, the Debye model and the Einstein model.

The Einstein model bases on the assumption that each atom as a harmonic oscillator vibrates along all three axes and all oscillators have the same frequency ω_0 this means the same energy $\hbar\omega_0$. The density of states can be written as

$$g_l(\omega) = 3n_a \delta(\omega - \omega_0) \quad (7)$$

where n_a [$1/m^3$] is the number of atoms per unit of volume, $\delta(\omega - \omega_0)$ is the Dirac function. Introducing (4), (7) into (3) one has

$$U_l = \int_{\omega_1}^{\omega_2} 3n_a \delta(\omega - \omega_0) \frac{1}{\exp\left(\frac{\hbar \omega}{k_B T_l}\right) - 1} \hbar \omega d\omega = \frac{3n_a \hbar \omega_0}{\exp\left(\frac{\hbar \omega_0}{k_B T_l}\right) - 1} \quad (8)$$

The phonon heat capacity using Einstein model can be expressed as

$$C_l = \frac{\partial U_l}{\partial T_l} = 3 n_a k_B \left(\frac{\bar{h} \omega_0}{k_B T_l} \right)^2 \frac{\exp\left(\frac{\bar{h} \omega_0}{k_B T_l}\right)}{\left[\exp\left(\frac{\bar{h} \omega_0}{k_B T_l}\right) - 1 \right]^2} \quad (9)$$

The Debye model assumes that all phonons of a particular mode, longitudinal or traverse, have a linear dispersion relation. This dispersion relation does not extend to infinity. The maximum frequency allowed by the Debye model is equal to [4]

$$\omega_D = c \left(\frac{6 \pi^2 N_l}{V} \right)^{\frac{1}{3}} \quad (10)$$

where c is the speed of sound and V is the given volume.

The density of states using Debye model can be expressed as [4]

$$g_l(\omega) = \frac{V}{2 \pi^2 c^3} \omega^2 \quad (11)$$

The Debye temperature is also introduced

$$T_D = \frac{\hbar \omega_D}{k_B} \quad (12)$$

In Table 1 the Debye temperature and melting temperature for selected metals are collected.

Using formulas (3), (11) the phonon thermal capacity can be calculated

$$C_l = \frac{\partial U_l}{\partial T_l} = \frac{V}{2 \pi^2 c^3} \int_0^{\omega_D} \frac{\partial f_{BE}(\omega, T_l)}{\partial T_l} \hbar \omega^3 d\omega \quad (13)$$

or

$$C_l = \frac{V \hbar^2}{2 \pi^2 c^3 k_B T_l^2} \int_0^{\omega_D} \omega^4 \frac{\exp\left(\frac{\hbar \omega}{k_B T_l}\right)}{\left[\exp\left(\frac{\hbar \omega}{k_B T_l}\right) - 1 \right]^2} d\omega \quad (14)$$

Table 1

The Debye temperature and melting temperature [7]

Metal	Number of atoms $n_a [10^{28}/\text{m}^3]$	Debye temperature $T_D [\text{K}]$	Melting temperature $T_m [\text{K}]$
Li	4.70	344	454
Na	2.65	158	371
Cu	8.45	340	1358
Ag	5.85	225	1235
Au	5.90	165	1338
Mg	8.60	400	922
Ca	4.60	230	1113
Zn	13.10	327	692
Fe	17.00	470	1811
Al	18.10	428	934
Sn	14.80	170	505
Pb	3.30	105	601
W	5.91	400	3695
Ti	13.80	420	1941

The following substitution is introduced

$$x = \frac{\hbar \omega}{k_B T_l} \quad (15)$$

and then

$$C_l = \frac{V k_B^4 T_l^3}{2\pi^2 c^3 \hbar^3} \int_0^{\frac{T_D}{T_l}} \frac{x^4 \exp(x)}{[\exp(x) - 1]^2} dx \quad (16)$$

Because $k_B/\hbar = \omega_D/T_D$ (c.f. equation (12)), so

$$C_l = \frac{V k_B}{2\pi^2 c^3} \omega_D^3 \left(\frac{T_l}{T_D}\right)^3 \int_0^{\frac{T_D}{T_l}} \frac{x^4 \exp(x)}{[\exp(x) - 1]^2} dx \quad (17)$$

or taking into account the formula (10)

$$C_l = 3 N_l k_B \left(\frac{T_l}{T_D} \right)^3 \int_0^{\frac{T_D}{T_l}} \frac{x^4 \exp(x)}{[\exp(x)-1]^2} dx \quad (18)$$

Finally

$$C_l = 9 n_a k_B \left(\frac{T_l}{T_D} \right)^3 \int_0^{\frac{T_D}{T_l}} \frac{x^4 \exp(x)}{[\exp(x)-1]^2} dx \quad (19)$$

where n_a [$1/m^3$] is the number of atoms per unit of volume.

It should be pointed out that the thermal capacity predicted by the Debye theory agrees very well with experimental data of many solids [7].

Notice that integration by parts leads to the formula

$$\int_0^{\frac{T_D}{T_l}} \frac{x^4 \exp(x)}{[\exp(x)-1]^2} dx = 4 \int_0^{\frac{T_D}{T_l}} \frac{x^3}{[\exp(x)-1]} dx - \frac{\left(\frac{T_D}{T_l} \right)^4}{\exp\left(\frac{T_D}{T_l} \right) - 1} \quad (20)$$

When T_l is essentially greater than Debye temperature T_D , then $T_D/T_l \rightarrow 0$ and $\exp(x) - 1 \approx x$. Thus

$$\int_0^{\frac{T_D}{T_l}} \frac{x^3}{[\exp(x)-1]} dx \approx \int_0^{\frac{T_D}{T_l}} x^2 dx = \frac{1}{3} \left(\frac{T_D}{T_l} \right)^3 \quad (21)$$

and the thermal capacity (19) is constant

$$C_l = 3 n_a k_B \quad (22)$$

For $T_l \ll T_D$ it can be assumed that $T_D/T_l \rightarrow \infty$ and then [7]

$$\int_0^{\infty} \frac{x^4 \exp(x)}{[\exp(x)-1]^2} dx = 4 \int_0^{\infty} \frac{x^3}{[\exp(x)-1]} dx = 4 \cdot 6 \frac{\pi^4}{90} \quad (23)$$

In this case the following approximation of thermal capacity can be accepted

$$C_l = \frac{12\pi^4}{5} n_a k_B \left(\frac{T_l}{T_D} \right)^3 \quad (24)$$

which is known as the T_l^3 law, and it agrees with experiments within a few percents for $T_l/T_D < 0.1$ [7].

In the general case the thermal capacity of phonons should be calculated directly from equation (19) using numerical methods.

In Figure 1 the course of lattice thermal capacity obtained from equation (19) for selected metals is shown. In this Figure the approximations (22) and (24) are also marked.

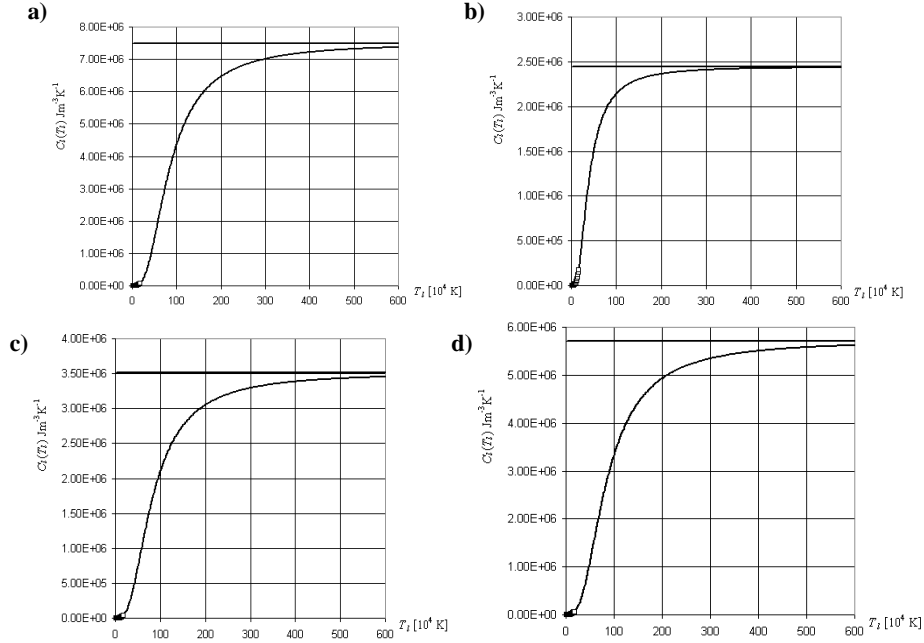


Fig. 1. Lattice thermal capacity $C_l(T_l)$: a) Al, b) Au, c) Cu, d) Ti

2. Phonons thermal conductivity

The phonons thermal conductivity of metals can be expressed as [5]

$$\lambda_l(T_l) = \frac{1}{3} C_l(T_l) \tau_{ph}(T_l) v_l^2 \quad (25)$$

where $C_l(T_l)$ is the lattice thermal capacity, $\tau_{ph}(T_l)$ is the total phonons scattering time and v_l is the speed of phonons. The equation (25) bases on the assumption that the phonons speed and the relaxation time are independent of frequency.

The thermal capacity $C_l(T_l)$ predicted by the Debye model is the function of temperature (c.f. equation (19)) and it is nearly constant at temperatures close to or higher than the Debye temperature (equation (22)). Additionally, using the Debye

model, the velocity v_l is assumed constant and equal to the speed of sound within material and then

$$\lambda_l(T_l) = n_a k_B c^2 \tau_{ph}(T_l) \quad (26)$$

Phonons collisions can occur with other phonons or defects. Using the Matthiessen rule [7, 8] one has

$$\frac{1}{\tau_{ph}} = \frac{1}{\tau_{ph\ ph}} + \frac{1}{\tau_{ph\ d}} \quad (27)$$

where $\tau_{ph\ ph}$ and $\tau_{ph\ d}$ are the phonon-phonon scattering time and phonon-defect scattering time, respectively.

The scattering time τ_{ph} is inversely proportional to the temperature at relatively high temperatures, while the phonon-defect scattering is typically independent of temperature. So, the thermal conductivity λ_l is inversely proportional to the temperature in the high-temperature limit [4, 7].

It should be pointed out that in numerical modelling of microscale heat transfer usually the constant lattice thermal conductivity is used $\lambda_l = \lambda_0$, where λ_0 is the thermal conductivity for $T_e = T_l$ at the room temperature [10, 11].

In the Table 2 the lattice thermal conductivity and heat capacity of selected metals are collected.

Table 2

Thermal conductivity λ_0 and thermal capacity C_l of selected metals [12]

Metal	Thermal conductivity λ_0 [$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$]	Thermal capacity C_l [$10^6\text{J}\cdot\text{m}^{-3}\cdot\text{K}^{-1}$]
Li	84.8	1.912
Na	142.0	1.380
Cu	409.0	3.390
Ag	429.0	2.620
Au	315.0	2.500
Mg	156.0	1.773
Ca	201.0	3.060
Zn	120.0	1.938
Fe	80.4	3.537
Al	237.0	2.422
Sn	6.66	4.450
Pb	35.3	1.440
W	174	3.000
Ti	21.9	2.340

3. Electron-phonon coupling factor

The electron-phonon coupling was first analyzed by Kaganov et al. [8]. In this model it is assumed that at lattice and electron temperatures much higher than the Debye temperature and $T_e \gg T_l$ the electron-lattice energy exchange rate can be expressed as

$$\frac{\partial E}{\partial t} = G(T_e)(T_l - T_e) \quad (28)$$

where

$$G(T_e) = \frac{\pi^2 m_e c^2 n_e}{6 \tau_e(T_e) T_e} \quad (29)$$

where c is the speed of sound, m_e is the effective electron mass, n_e is the number density of electrons, $\tau_e(T_e)$ is the electron relaxation time defined as the electron-phonon scattering time $\tau_{e\text{ ph}}(T_e)$ evaluated under the assumption that the lattice temperature is equal to the electron temperature, $G(T_e)$ is the electron-phonon coupling factor. The electron-phonon scattering time $\tau_{e\text{ ph}}(T_e)$ is inversely proportional to the lattice temperature $1/T_e$ and then one obtains the constant value of coupling factor

$$G = \frac{\pi^2 m_e c^2 n_e}{6 A} \quad (30)$$

where A is the constant.

Although a constant value for the electron-phonon coupling factor is used in most of the current computational and theoretical investigations of short pulse laser interactions with metals films, there is growing experimental evidence suggesting that the constant electron-phonon coupling factor may be limited to low laser intensities, this means low electrons temperatures [8].

For high electrons temperatures a simple expression for the temperature dependent electron-phonon coupling factor can be used [8]

$$G(T_e) = \frac{\pi \hbar k_B l \langle \omega^2 \rangle}{g(E_F)} \int_{-\infty}^{\infty} g^2(E) \left(-\frac{\partial f(E, \mu, T_e)}{\partial E} \right) dE \quad (31)$$

where $g(E)$ is the electron density of states (DOS) at the energy level E , $f(E, \mu, T_e)$ is the Fermi distribution function [7], l is the electron-phonon mass enhancement parameter [8] and $\langle \omega^2 \rangle$ is the second moment of the phonon spectrum defined by McMillan [8].

At very low electrons temperatures $\partial f / \partial E$ reduces to the Dirac function ($E \rightarrow E_F$)

$$\int_{-\infty}^{\infty} g^2(E) \left(-\frac{\partial f(E, \mu, T_e)}{\partial E} \right) dE = \int_{-\infty}^{\infty} g^2(E) \delta(E - E_F) dE = g^2(E_F) \quad (32)$$

and then the electron-phonon coupling factor is constant

$$G(T_e) = G_0 = \pi \hbar k_B l \langle \omega^2 \rangle g(E_F) \quad (33)$$

Finally, the formula (31) can be written as follows

$$G(T_e) = \frac{G_0}{g^2(E_F)} \int_{-\infty}^{\infty} g^2(E) \left(-\frac{\partial f(E, \mu, T_e)}{\partial E} \right) dE \quad (34)$$

and for high electrons temperatures this dependence should be used. In Table 3 the values of l , $\langle \omega^2 \rangle$ and G_0 for selected metals are collected.

Table 3

The electron-phonon coupling constant l , the value of $\langle \omega^2 \rangle$ and the constant coupling factor G for selected metals [8]

Metal	Electron-phonon coupling constant l	The value of $\langle \omega^2 \rangle$	The constant coupling factor G [$\text{Wm}^{-3}\text{K}^{-1}$]
Al	0.45	185.9	$2.45 \cdot 10^{17}$
Ag	0.12	22.5	$0.25 \cdot 10^{17}$
Cu	0.13	29 ± 4	$1.00 \cdot 10^{17}$
Au	0.17	23 ± 4	$0.25 \cdot 10^{17}$
Ni	0.084	49.5	$3.60 \cdot 10^{17}$
Pt	0.66	142.5	$2.50 \cdot 10^{17}$
W	0.28	112 ± 15	$5.00 \cdot 10^{17}$
Ti	0.38	350 ± 30	$1.00 \cdot 10^{19}$

In Figure 2 the course of electron-phonon coupling factor for selected metals is shown. The data have been taken from [9]. In this Figure the constant value of G is also marked.

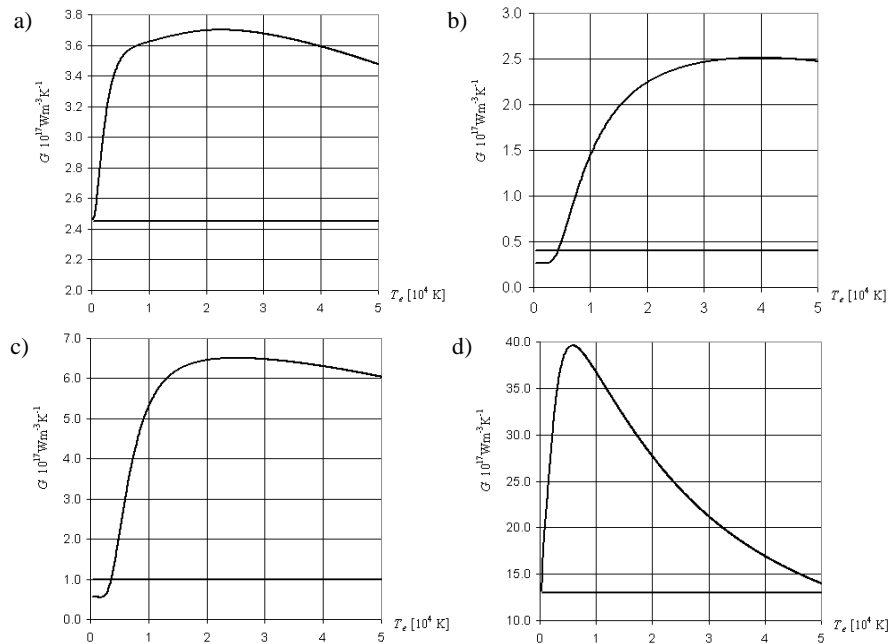


Fig. 2. Electron-phonon coupling factor: a) Al, b) Au, c) Cu, d) Ti

Conclusions

Two-temperature microscale heat transfer model is presented. The ways assuring the determination of thermophysical parameters are discussed. In particular, the free electron gas model is used to describe temperature dependent electrons thermophysical parameters and the phonons gas model is applied to describe the lattice thermophysical parameters. The temperature dependent electron-phonon coupling factor is also determined.

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