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Heat Transfer by Phonons in Landauer-Datta-Lundstrom Approach

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The Landauer-Datta-Lundstrom generalized transport model is applied to heat transfer by phonons. In both cases of electrons and phonons the Landauer approach generalized and extended by Datta and Lundstom gives correct quantitative description of transport processes for resistors of any dimension and size in ballistic, quasi-ballistic, and diffusive linear response regimes when there are differences in both voltage and temperature across the device. It is shown that the lattice thermal conductivity can be written in a form that is very similar to the electrical conductivity. Important differences between electrons and phonons are discussed.

Keywords: Nanoelectronics, Conduction modes, Transmission coefficient, Ballistic transport, Heat transport, Phonon transport.

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1. INTRODUCTION

Electrons transfer both charge and heat. Electrons carry most of the heat in metals. In semiconductors electrons carry only a part of the heat but most of the heat is carried by phonons.

The objectives for this short report is to give a condensed summary of Landauer-Datta-Lundstrom (LDL) transport model [1-4] to describe the phonon heat flux which works at the nanoscale as well as at macroscale for 1D, 2D, and 3D resistors in ballistic and diffusive linear response regimes.

The phonon heat flux is proportional to the temperature gradient

$$J_{Qx}^{ph} = -\kappa_L \frac{dT}{dx} \ [W/m^2] \qquad (1)$$

with coefficient κ_L known as the specific lattice thermal conductivity. Such an exceptional thermal conductor like diamond has $\kappa_L \approx 2 \cdot 10^3 \ W/m \cdot K$ while such a poor thermal conductor like glass has $\kappa_L \approx 1 W/m \cdot K$. Note that electrical conductivities of solids vary over more than 20 orders of magnitude, but thermal conductivities of solids vary over a range of only 3-4 orders of magnitude. We will see that the same methodology used to describe electron transport can be also used for phonon transport. We will also discuss the differences between electron and phonon transport. For a thorough introduction to phonons use classical books [5-8].

2. HEAT TRANSFER BY PHONONS

To describe the phonon current we need an expression like for the electron current

$$I = \frac{2q}{h} \int T_{el}(E) M_{el}(E) \left(f_1 - f_2 \right) dE \, . \qquad (2)$$

For electrons the states in the contacts were filled according to the equilibrium Fermi functions, but phonons obey Bose statistics, thus the phonon states in the contacts are filled according to the equilibrium Bose – Einstein distribution

$$n_0(\hbar\omega) = \frac{1}{e^{\hbar\omega/kT} - 1} \, . \qquad (3)$$

Let temperature for the left and the right contacts are T_1 and T_2. As for the electrons, both contacts are assumed ideal. Thus the phonons that enter a contact are not able to reflect back, and transmission coefficient $T_{ph}(E)$ describes the phonon transmission across the entire channel.

It is easy now to rewrite eqn. (2) to the phonon heat current. Electron energy E we replace to the phonon energy $\hbar\omega$. In the electron current we have charge q moving in the channel, in case of the phonon current the quantum of energy $\hbar\omega$ is moving instead; thus, we replace q in (2) with $\hbar\omega$ and move it inside the integral. The coefficient 2 in (2) reflects the spin degeneracy of an electron. In case of the phonons we remove this coefficient, and instead the number of the phonon polarization states that contribute to the heat flow let us include to the number of the phonon modes $M_{ph}(\hbar\omega)$. Finally, the heat current due to phonons is

$$Q = \frac{1}{h} \int (\hbar\omega) T_{ph}(\hbar\omega) M_{ph}(\hbar\omega) \left(n_1 - n_2 \right) d(\hbar\omega) \, . \qquad (4)$$

In the linear response regime

$$n_1 - n_2 \approx -\frac{\partial n_0}{\partial T} \Delta T \, , \qquad (5)$$

where the derivative according (3)

$$\frac{\partial n_0}{\partial T} = \frac{\hbar\omega}{T} \left(-\frac{\partial n_0}{\partial (\hbar\omega)} \right) , \qquad (6)$$

with

$$\frac{\partial n_0}{\partial(\hbar\omega)} = \left(-\frac{1}{kT}\right)\frac{e^{\hbar\omega/kT}}{(e^{\hbar\omega/kT}-1)^2}. \quad (7)$$

Now eqn (4) for small differences in temperature becomes

$$Q = -K_L \Delta T, \quad (8)$$

where the thermal conductance

$$K_L = \frac{k^2 T}{h}\int T_{ph}(\hbar\omega) M_{ph}(\hbar\omega)\left[\left(\frac{\hbar\omega}{kT}\right)^2\left(-\frac{\partial n_0}{\partial(\hbar\omega)}\right)\right] d(\hbar\omega) \quad (9)$$

Equation (8) is simply the Fourier's law stating that heat flows down to a temperature gradient. It is also useful to note that the thermal conductance (9) displays certain similarities with the electrical conductance

$$G = \frac{2q^2}{h}\int T_{el}(E) M_{el}(E)\left(-\frac{\partial f_0}{\partial E}\right) dE. \quad (10)$$

The derivative

$$W_{el}(E) \equiv \left(-\frac{\partial f_0}{\partial E}\right) \quad (11)$$

known as the Fermi window function that cutting out those conduction modes which only contribute to the electric current. The electron windows function is normalized:

$$\int_{-\infty}^{+\infty}\left(-\frac{\partial f_0}{\partial E}\right) dE = 1. \quad (12)$$

In case of phonons the term in square brackets of eqn (9) acts as a window function to specify which modes carry the heat current. After normalization

$$W_{ph}(\hbar\omega) = \frac{3}{\pi^2}\left(\frac{\hbar\omega}{kT}\right)\left(\frac{\partial n_0}{\partial(\hbar\omega)}\right); \quad (13)$$

thus finally

$$K_L = \frac{\pi^2 k^2 T}{3h}\int T_{ph}(\hbar\omega) M_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega) \quad (14)$$

with

$$g_0 \equiv \pi^2 k^2 T / 3h \approx (9.456\times 10^{-13}\ W/K^2)T, \quad (15)$$

known as the quantum of thermal conductance experimentally observed first in 2000 [9].

Comparing eqns (10) and (14) one can see that the electrical and thermal conductances are similar in structure: both are proportional to corresponding quantum of conductance times an integral over the transmission times the number of modes times a window function.

The thermal broadening functions for electrons and phonons have similar shapes and each has a width of a few kT. In case of electrons this function is

$$F_T(x) \equiv \frac{e^x}{\left(e^x+1\right)^2} \quad (16)$$

with $x \equiv (E-\mu)/kT$. This function for phonons is given by eqn (13) or

$$F_T^{ph}(x) \equiv \frac{3}{\pi^2}\frac{x^2 e^x}{\left(e^x-1\right)^2} \quad (17)$$

with $x \equiv \hbar\omega/kT$. Both functions are normalized to a unity and shown together on fig. 1.

Along with the number of modes determined by the dispersion relation, these two window functions play a key role in determining the electrical and thermal conductances.

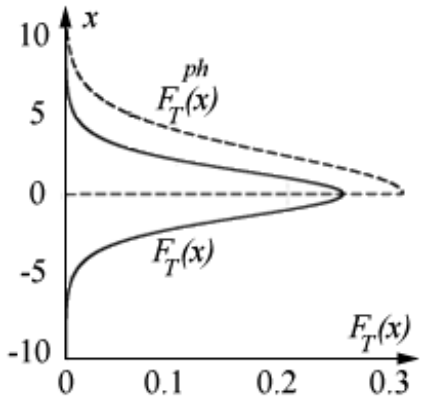

Fig. 1 – Broadening function for phonons compared to that of electrons

2.1 Thermal Conductivity of the Bulk Conductors

The thermal conductivity of a large diffusive resistor is a key material property that controls performance of any electronic devices. By analogy with the transmission coefficient for electron transport the phonon transmission

$$T_{ph}(\hbar\omega) = \frac{\lambda_{ph}(\hbar\omega)}{\lambda_{ph}(\hbar\omega)+L}\Big|_{L\gg\lambda_{ph}} \to \frac{\lambda_{ph}(\hbar\omega)}{L}. \quad (18)$$

It is also obvious that for large 3D conductors the number of phonon modes is proportional to the cross-sectional area of the sample:

$$M_{ph}(\hbar\omega) \propto A, \quad (19)$$

Now let us return to eqn (8) dividing and multiplying it by A/L, which immediately gives eqn (1) for the phonon heat flux postulated above

$$\frac{Q}{A} \equiv J_{Qx}^{ph} = -\kappa_L \frac{dT}{dx} \quad (20)$$

with specific lattice thermal conductivity

$$\kappa_L = K_L \frac{L}{A}, \tag{21}$$

or substituting (18) to (14) one for the lattice thermal conductivity finally obtains

$$\kappa_L = \frac{\pi^2 k^2 T}{3h} \int \frac{M_{ph}(\hbar\omega)}{A} \lambda_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega). \tag{22}$$

It is useful now to define the average number of phonon modes per cross-sectional area of the conductor that participate in the heat transport

$$\left\langle M_{ph} / A \right\rangle \equiv \int \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega)\, d(\hbar\omega). \tag{23}$$

Then

$$\kappa_L = \frac{\pi^2 k^2 T}{3h} \left\langle M_{ph} / A \right\rangle \left\langle\left\langle \lambda_{ph} \right\rangle\right\rangle, \tag{24}$$

where the average mean-free-path is defined now as

$$\left\langle\left\langle \lambda_{ph} \right\rangle\right\rangle = \frac{\int \frac{M_{ph}(\hbar\omega)}{A} \lambda_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega)}{\int \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega)\, d(\hbar\omega)}. \tag{25}$$

Thus, the couple of the phonon transport equations (20) and (24) corresponds to similar electron transport equations:

$$J_x = \frac{\sigma}{q} \frac{d\left(E_F\right)}{dx}, \tag{26}$$

$$\sigma = \frac{2q^2}{h} \left\langle M_{el} / A \right\rangle \left\langle\left\langle \lambda_{el} \right\rangle\right\rangle. \tag{27}$$

The thermal conductivity (24) and the electrical conductivity (27) have the same structure. It is always a product of the corresponding quantum of conductance times the number of modes that participate in transport, times the average mean-free-path. These three quantities for phonons will be discussed later.

2.2 Specific Heat Versus Thermal Conductivity

The connection between the lattice specific thermal conductivity and the lattice specific heat at constant volume is well known [5-8]. We will show now that corresponding proportionality coefficient is a product of an appropriately-defined mean-free-path $\left\langle\left\langle \Lambda_{ph} \right\rangle\right\rangle$ and an average phonon velocity $\left\langle v_{ph} \right\rangle$, namely:

$$\kappa_L = \frac{1}{3} \left\langle\left\langle \Lambda_{ph} \right\rangle\right\rangle \left\langle v_{ph} \right\rangle C_V. \tag{28}$$

The total phonon energy per unit volume

$$E_{ph} = \int_0^\infty (\hbar\omega) D_{ph}(\hbar\omega)\, n_0(\hbar\omega)\, d(\hbar\omega), \tag{29}$$

where $D_{ph}(\hbar\omega)$ is the phonon density of states. By definition,

$$\begin{aligned} C_V &\equiv \frac{\partial E_{ph}}{\partial T} = \frac{\partial}{\partial T} \int_0^\infty (\hbar\omega) D_{ph}(\hbar\omega)\, n_0(\hbar\omega)\, d(\hbar\omega) = \\ &= \int_0^\infty (\hbar\omega) D_{ph}(\hbar\omega) \left(\frac{\partial n_0(\hbar\omega)}{\partial T} \right) d(\hbar\omega) = \\ &= \frac{\pi^2 k^2 T}{3} \int_0^\infty D_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega) \end{aligned} \tag{30}$$

where eqns (6) and (13) were used. Next, multiply and divide (22) by (30) and obtain proportionality we are looking for:

$$\kappa_L = \left[\frac{\frac{1}{h} \int_0^\infty \frac{M_{ph}(\hbar\omega)}{A} \lambda_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega)}{\int_0^\infty D_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega)} \right] C_V. \tag{31}$$

To obtain final expression (28) and correct interpretation of the proportionality coefficient we need to return to eqn (18). This expression can be easily derived for 1D conductor with several simplifying assumptions. Nevertheless it works very well in practice for a conductor of any dimension. Derivation of eqn (18) is based on the interpretation of the mean-free-path $\lambda(E)$ or $\lambda(\hbar\omega)$ as that its inverse is the probability per unit length that a positive flux is converted to a negative flux. This is why λ is often called a mean-free-path for backscattering. Let us relate it to the scattering time τ. The distinction between mean-free-path and mean-free-path for backscattering is easiest to see for 1D conductor. Let electron undergoes a scattering event. For isotropic scattering the electron can forward scatter or back scatter. Only backscattering is relevant for the mean-free-path for scattering, so the time between backscattering events is 2τ. Thus the mean-free-path for backscattering is twice the mean-free-path for scattering

$$\lambda_{1D}(E) = 2\Lambda(E) = 2v(E)\tau(E). \tag{32a}$$

It was shown that the proper definition of the mean-free-path for backscattering for a conductor of any dimension [10]

$$\lambda(E) = 2 \frac{\left\langle v_x^2 \tau \right\rangle}{\left\langle | v_x | \right\rangle},$$

where averaging is performed over angles. For isotropic bands

$$\lambda_{2D}(E) = \frac{\pi}{2} v(E)\,\tau(E)\,, \qquad (32b)$$

$$\lambda_{3D}(E) = \frac{4}{3} v(E)\,\tau(E)\,. \qquad (32c)$$

The scattering time is often approximately written as the power law scattering

$$\tau(E) = \tau_0 \left(\frac{E - E_C}{kT} \right)^s , \qquad (33)$$

where exponent s describes the specific scattering mechanism: for acoustic phonon scattering in 3D conductor with parabolic dispersion $s = -1/2$, and for ionized impurity scattering $s = +3/2$ [11].

Analogous power law is often used for mean-free-path:

$$\lambda(E) = \lambda_0 \left(\frac{E - E_C}{kT} \right)^r . \qquad (34)$$

For parabolic zone structure $v(E) \propto E^{1/2}$, thus $r = s + 1/2$ with $r = 0$ for acoustic phonon scattering, and $r = 2$ for ionized impurity scattering.

Coming back to our initial task to derive (28) from (31) for 3D conductor according (32c) we have

$$\lambda_{ph}(\hbar\omega) = \frac{4}{3} v_{ph}(\hbar\omega)\,\tau_{ph}(\hbar\omega)\,, \qquad (35)$$

where according to (32a),

$$v_{ph}(\hbar\omega)\,\tau_{ph}(\hbar\omega) = \Lambda_{ph}(\hbar\omega)\,, \qquad (36)$$

and finally

$$\lambda_{ph}(\hbar\omega) = \frac{4}{3} \Lambda_{ph}(\hbar\omega)\,. \qquad (37)$$

It is known that the density of states and number of modes for electrons in 3D:

$$M_{el}(E) = AM_{3D}(E) = A\frac{h}{4} \left\langle v_x^+(E) \right\rangle D_{3D}(E)\,. \qquad (38)$$

Let us rewrite this formulae for phonons. Note that the spin degeneracy for electrons $g_s = 2$ is included to the density of states

$$D_{3D}(E) = 2D'_{3D}(E)\,, \qquad (39)$$

and for spherical bands in 3D conductor

$$\left\langle v_x^+(E) \right\rangle = \frac{v_{el}(E)}{2}\,. \qquad (40)$$

Collecting (38) up to (40) all together in case of phonons we have

$$M_{ph}(\hbar\omega) = A\frac{h}{2} \left(\frac{v_{ph}(\hbar\omega)}{2} \right) 2D_{ph}(\hbar\omega) = \\ = A\frac{h}{4} v_{ph}(\hbar\omega) D_{ph}(\hbar\omega) \qquad (41)$$

Substituting (37) and (41) to (31) we obtain

$$\kappa_L = \left[\frac{\frac{1}{3}\int_0^\infty \Lambda_{ph}(\hbar\omega)\, v_{ph}(\hbar\omega) D_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega)}{\int_0^\infty D_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega)} \right] C_V\,. \qquad (42)$$

Multiplying and dividing (42) by

$$\int_0^\infty v_{ph}(\hbar\omega) D_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega)\,, \qquad (43)$$

we finally get eqn (28) with proportionality coefficient between κ_L and C_V as the product of an average mean-free-path as

$$\left\langle\left\langle \Lambda_{ph} \right\rangle\right\rangle \equiv \frac{\int_0^\infty \Lambda_{ph}(\hbar\omega)\, v_{ph}(\hbar\omega) D_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega)}{\int_0^\infty v_{ph}(\hbar\omega) D_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega)} \qquad (44)$$

and an average velocity as

$$\left\langle v_{ph} \right\rangle \equiv \frac{\int_0^\infty v_{ph}(\hbar\omega) D_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega)}{\int_0^\infty D_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega)}\,, \qquad (45)$$

with the appropriate averaging.

Equation (28) is often used to estimate the average mean-free-path from the measured κ_L and C_V, if we know the average velocity, which is frequently assumed to be the longitudinal sound velocity. The derivation above has identified the precise definitions of the $\left\langle\left\langle \Lambda_{ph} \right\rangle\right\rangle$ and $\left\langle v_{ph} \right\rangle$. If a phonon dispersion is chosen one can always compute the average velocity according to (45), and it is typically very different from the longitudinal sound velocity. Thus, estimates of the average mean-free-path can be quite wrong if one assumes the longitudinal sound velocity [12].

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