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Effective interface thermal resistance and thermal conductivity of dielectric nanolayers

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ABSTRACT

Analytical expressions for the effective interface thermal resistance (ITR) and thermal conductivity k of dielectric nanolayers are derived and analyzed, based on the analytical solution of the phonon Boltzmann transport equation under the gray relaxation time approximation. This is achieved by using accurate expressions for the temperature and one-dimensional heat flux propagating across nanolayers supporting a diffusive phonon scattering at their interfaces. It is shown that the effective ITR between two layers can be symmetric on their thermal properties, such that its asymptotic value in the ballistic regime is higher than that in the diffusive one. In the ballistic-diffusive regime, the effective ITR depends strongly on the ratio $\lambda = L/l$, between the layer thickness L and mean free path l of phonons. Our predictions for the effective ITR in the ballistic regime are in good agreement with those of the diffuse mismatch model, while they differ by about 16% in the diffusive regime. On the other hand, k increases with λ until reaching saturation for bulk layers and agrees rather well with previous predictions reported in the literature. The obtained results could be useful for analytically describing the heat transport in dielectric nanothin films and superlattices, in which the gray approximation is valid.

1. Introduction

In recent years, the thermal transport in thin solid films with thickness ranging from tens of nanometers to micrometers has become an important research topic in fundamental science [1–4], due to its importance and potential applications in electronics and photonics [5]. As is well known, when the thickness of a thin film becomes comparable to the mean free paths (MFP) of its heat carriers (phonons and/or electrons) [6], heat conduction deviates from the predictions of the diffusive Fourier's law, due to their ballistic dynamics described by the Boltzmann transport equation (BTE) [7,8]. Significant efforts have been devoted to analytically and numerically solve the BTE, whose solution is rather difficult to determine, owing to its high dimensionality. Fuchs and Sondheimer derived analytical solutions of the BTE for electrons undergoing partially specular and partially diffuse boundary scattering [9,10]. Mazumder and Majumdar used a Monte-Carlo method to study the phonon transport along a silicon thin film including phonon dispersion and polarizations [11]. Based on the discrete-ordinates method and the gray relaxation time approximation, Majumdar numerically solved the BTE for the temperature and heat flux in a dielectric thin film, considering that its two surfaces are black phonon emitters [7]. More recently, Chen [12] obtained an implicit solution of the BTE to study the ballistic phonon transport in the cross-plane direction of superlattices and analyzed the inconsistent definitions of temperature at the interfaces. Chengyun [13] derived a semi-analytical solution of the frequency-dependent transient BTE using the method of degenerate kernels to study phonon transport in both the diffusive to ballistic regimes. More recently, a recent paper by Ordonez-Miranda et al. [14] presented explicit analytical solutions of the phonon BTE under the gray relaxation time approximation for the steady-state and modulated components of the temperature of dielectric layered systems. In this latter work, the effects of the interface mismatch are taken into account through the reflectivity and transmissivity of phonons, without involving the effective interface thermal resistance (ITR).

Two common models for estimating the effective ITR are the acoustic mismatch model (AMM) and the diffusive mismatch model (DMM) [15,16]. In the DMM, the incident phonon loses all memory of its direction and polarization, after being reflected or transmitted at the interface, while in the AMM, its direction of propagation is controlled by laws similar to those of Snell-Descartes in geometric optics. The AMM can explain experimental data for specular interfaces mainly, but fails to describe the heat transport across diffusive interfaces [15,17], which are better described by the DMM [18]. As the thickness of a dielectric thin film reduces to values comparable or smaller than the phonon MFP, size effects are expected to appear on the effective ITR, as is the case of its effective thermal conductivity [19–21]. This is the case

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Table 1
Room-temperature properties for the bulk semiconductor crystals considered in the analysis of dielectric layered systems. Data are obtained from Ref. [32].

Material	Density	Group velocity*	Specific heat	Bulk thermal	MFP**
	(kg/m^3)	(m/s)	(J/kg.K)	conductivity (W/m.K)	(nm)
Si	2329	2169	700	130	110
Ge	5323	1302	310	58	81
GaAs	5320	1237	330	55	76
InAs	5680	982	250	27	58
GaN	6150	1840	490	130	70
GaP	4140	1522	430	110	122
InP	4810	1152	310	68	119
InSb	5770	856	200	18	55

* The values correspond to the effective group velocities of phonons.
** Calculated using the kinetic theory $k_0 = \rho c v l/3$.

of nanothin films, in which the heat transport across their interfaces is still poorly understood [1]. Based on the two-temperature model of heat conduction, Ordonez-Miranda et al. [22] showed that both the effective thermal conductivity and ITR of metal-nonmetal layers depends strongly on the layer thicknesses. This size dependence was also confirmed by Yanbao Ma [23], who developed an analytical model for the effective thermal conductivity of dielectric thin films, through a non-Fourier heat transport approach. More recently, Jan Kaiser et al. [24] showed that the Fourier's law can still be used to describe the steady-state heat transport in dielectric nanostructures supporting ballistic heat transport, under appropriate boundary conditions at the interfaces. They also showed that the maximum deviation between the analytical solution of the BTE reported by Ordonez-Miranda et al. [14] and predictions of the Fourier's law for the semi-infinite layer is less than 16%.

The objective of the present work is to show that the analytical solutions of the phonon BTE obtained under the gray relaxation time approximation for the steady-state one-dimensional heat conduction in dielectric layered systems, can conveniently be rewritten under a more manageable “Fourier-like”form. This is done by replacing the reflectivity and transmissivity of phonons by the macroscopic concepts of effective ITR and thermal conductivity.

2. Solution for the steady-state heat conduction

The starting point of our analysis is one dimensional solution of the phonon BTE for the steady-state heat conduction inside a dielectric layer in thermal contact with a semi-infinite substrate, as shown in Fig. 1(a). The normalized temperature $U_n(x)$ and normalized heat flux Q_{sn} along the z-direction of layer $n = 1; 2$ are given by Ref. [14]:

$$2U_1(x) = E_2(x) + \int_0^{\lambda} U_1(x')E_1(|x - x'|)dx', \tag{1a}$$

$$2U_2(x) = E_2(x) + \int_0^{\infty} U_2(x')E_1(|x - x'|)dx', \tag{1b}$$

$$\frac{Q_{s1}}{2} = E_3(x) - \frac{d}{dx}\int_0^{\lambda} U_1(x')E_3(|x - x'|)dx', \tag{1c}$$

$$\frac{Q_{s2}}{2} = E_3(x) - \frac{d}{dx}\int_0^{\infty} U_2(x')E_3(|x - x'|)dx', \tag{1d}$$

where $x = z/l_1$ is the normalized position, l_1 is the gray MFP of phonons, $\lambda = L/l_1$ is the normalized layer thickness, τ_1 is the relaxation time of phonons, $E_n(x)$ is the exponential integral function of order n defined as [25]:

$$E_n(t) = \int_0^1 \mu^{n-2} e^{-t/\mu} d\mu, \tag{2}$$

and

$$U_n(x) = \frac{\pi I_{0n}(x) - A_n^-}{A_n^+ - A_n^-}, \tag{3a}$$

$$Q_{sn}(x) = \frac{q_0(x)}{A_n^+ - A_n^-}, \tag{3b}$$

I_{0n} being the steady-state component of the equilibrium phonon intensity, q_0 is the heat flux and the constants $A_n^{\pm}$ with $A_2^- = 0$ are determined by the boundary conditions. Eqs. (1a)-(1d) were derived assuming that the MFP (l) and relaxation time (τ) of phonons are both independent of temperature and well represented by their average values within all the spectral frequencies (gray-medium approximation). The first of these assumptions is valid for problems involving weak temperature gradients [26–28], while the second one holds for heat conduction driven by frequency-independent phonon-phonon scattering [6], as is the case for the ballistic regime considered in this work. Equations (1a)-(1d) for the temperature and conductive heat flux also hold for their radiative counterparts and their analytical solutions were reported by Modest [29] for the pure diffusive and pure ballistic regimes. However, in the intermediate diffusive-ballistic regime, Modest only reported numerical solutions, whose predictions agree quite well with the analytical ones derived by Ordonez-Miranda et al. [14]. According to the principle of energy conservation, the parameters $A_n^{\pm}$ are given by

$$\frac{A_2^+}{t_{12}} = \frac{A_1^-}{r_{12}}, \tag{4a}$$

$$A_1^+ = q_0 + 2A_1^- E_3(\lambda) + 2\int_0^{\lambda} \pi I_{01}(x)E_2(x)dx, \tag{4b}$$

where r_{ij} and t_{ij} are the energy reflectivity and transmissivity of phonons coming from the layer i to the layer j, respectively. For rough interfaces, as is usually the case in practice, phonons completely diffuse in all directions at the interface and these two parameters can be estimated by the phonon diffusive model [15], which establishes that [12]:

$$t_{ij} = r_{ji} = 1 - t_{ji} = \frac{\rho_j c_j v_j}{\rho_i c_i v_i + \rho_j c_j v_j}, \tag{5}$$

where ρ is the mass density, c is the specific heat, and v is the magnitude of the phonon group velocity. Equation (5) was applied by Chen [12] and Alvarez [18] to describe experimental data for the in-plane and cross-plane thermal conductivities of superlattices.

Given that exact analytical solutions of Eqs. (1a)-(1d) do not exist yet, they were analytically solved under a reasonable first-order approximation [14]. To quantify the accuracy of the solutions thus derived, we are going to use these previous results to solve Eqs. (1a)-(1d) for a second-order approximation, before studying in detail the heat transport in and across nanolayers. Under a first-order approximation, the analytical solutions $U_n^{(1)}(x) = U_n(x)$ of Eqs. (1a)-(1d) are given by Ref. [14].

$$U_1^{(1)}(x) = 1 - \alpha[x + \beta + \gamma(p(x) - p(\lambda - x))], \tag{6a}$$

$$\alpha = \frac{3}{4}Q_{s1} = \frac{1}{\lambda + 2\beta}, \tag{6b}$$

$$U_2^{(1)} = 1 - \frac{3}{4}Q_{s2}(x + p(x)), \tag{6c}$$

where the parameters β and γ can be determined by evaluating Eqs. (1a) and (1c) at $x = 0$ in combination with Eqs. (6a) and (6b). The final results are

$$\beta(\lambda) = \frac{\xi(1/3 + E_4(\lambda)) + C_2(1/2 - E_3(\lambda))}{C_2(1 - E_2(\lambda)) + \xi(1/2 + E_3(\lambda))}, \tag{7a}$$

$$\gamma(\lambda) = \frac{(1 - E_2(\lambda))(1/3 + E_4(\lambda)) - (1/4 - E_3^2(\lambda))}{C_2(1 - E_2(\lambda)) + \xi(1/2 + E_3(\lambda))}, \tag{7b}$$

with $\xi = C_1 + 2(p(\lambda) - p(0))$, $C_n = \int_0^{\lambda}(p(x) - p(\lambda - x))E_n(x)dx$, and