Statistical model of phonon scattering on rough boundaries of nanostructures

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Abstract. Because of the rapid development of semiconductor electronics and the tendency to size reduction of the elements of transistors, there is an urgent task of assessing the heat transfer regime, which determines the ability to maintain the required thermal regime. In this work, the heat transfer in micro- and nanostructures in silicon is considered, and a comprehensive analysis of factors determining the heat transfer regime is carried out. In particular, the effect of the interaction of phonons with the sample boundaries in the quasi-ballistic and ballistic heat transfer regimes, where these processes play a decisive role, is evaluated using statistical model of phonon scattering on rough boundaries of samples.

1. Introduction
Modern technologies for the development and production of semiconductor structures are based on micro- and nanoscale elements. At the same time, the functioning of electronic components in the estimating conditions is impossible without maintaining the required thermal regime, since severe restrictions are imposed by the operating temperature range [1]. In contrast to macroscopic bodies, for which the classical laws of heat transfer are applicable, in micro- and nanoscale structures, it is necessary to use completely different methods based on statistics of quasiparticles, i.e., phonons being quanta of lattice vibrations, taking into account the so-called size effect.

At the moment, the problem of heat propagation in solids is well studied. In this case, the classical theory of thermal conductivity considers objects with characteristic size much exceeding the mean free path of heat carriers, . In other words, by introducing a dimensionless parameter, the Knudsen number , it may be argued that the existing theory of thermal conductivity, based on Fourier's law, is applicable for the values in the diffusion transport regime.

Current trends in the development of solid-state semiconductor structures based on micro- and nanoscale elements require the study of heat transfer processes under conditions when the processes of interaction of phonons with the sample boundary begin to play a significant or decisive role in thermal conductivity [2]. This circumstance essentially distinguishes the transfer process from the diffusion regime, where the main processes are the interaction of phonons with each other (transfer processes), and the influence of the boundaries is noticeable only at temperatures much lower than the Debye temperature [3]. In this regard, two regimes of heat transfer are distinguished [4]:

1. the ballistic regime, , when the mean free path of the heat carriers – phonons – is much larger than the characteristic size of the sample; phonons almost do not interact with each other, freely
propagate inside the structure and are scattered at the sample boundary (or at the interface in the case of superlattices);

2. diffusion-ballistic, $Kn \sim 1$, when part of the phonons is involved in the ballistic transfer, and the other part is involved in the diffusion, which corresponds to the classical law of thermal conductivity in a macroscopic sample.

At the moment, a calculation method with sufficient predictive power that allows to effectively control the thermal regime, has not been found yet [4]. Therefore, the purpose of this work is a comprehensive analysis of the processes of interaction of phonons with the sample boundary by the example of Silicon, and identification of factors that affect the process of heat transfer in the ballistic and diffusion-ballistic regimes. Moreover, the solution of this task plays a significant role in phonon-boundary collisions on rough surfaces, such as free boundaries [3] and interfaces [5,6].

2. Evaluation of the heat transfer regime

As shown earlier, the heat transfer regimes can be estimated using the Knudsen number. In this case, it is necessary to take into account that the free path of the phonon $l$ depends on the temperature $T$, the energy of the phonon (phonon frequency $\omega$) and its polarization $j$, that is, the problem is multiparametric, so $l = l(j, \omega, T)$. In order to minimize the number of significant parameters, we estimate the average free path $ar{l}$ through the equation for thermal conductivity, obtained on the basis of the solution of the Boltzmann transport equation in the relaxation time approximation and data on the lattice dynamics (dispersion curves and free path times of phonons) [7,3].

$$k_{\text{bulk}}(T) = \frac{1}{3} \sum_{j=1}^{\text{max}, \text{min}, 0} \int_{0}^{\infty} \frac{df_{j}(\omega, T)}{d\omega} D_{j}(\omega) v_{\text{g},j}(\omega) l_{j}(\omega, T) d\omega,$$

where $j$ is the polarization of the phonon wave ($j = 1$ corresponds to the transverse TA wave, and $j = 2$ corresponds to the longitudinal LA), $f_{j}$ is the Bose-Einstein equilibrium distribution function; $D_{j}$ is the density of the states (DOS) of the phonons with polarization $j$; $v_{\text{g},j}$ is the group velocity of the phonons; and $l_{j}$ is the mean free path of the phonons, which is determined according to the Matthiessen rule as a result of all interaction processes:

$$l^{-1}(j, \omega, T) = l_{\text{ph-ph}}^{-1}(j, \omega, T) + l_{\text{imp}}^{-1}(j) + l_{\text{bound}}^{-1}(j, \omega).$$

Here $l_{\text{ph-ph}}$ is the mean free path between phonon-phonon interactions, determined, for example, by the approach [8] (figure 1); $l_{\text{imp}}$ is the path length between successive interactions of phonons with lattice inhomogeneities (impurity atoms, etc.); and $l_{\text{bound}}$ is the mean free path of the phonons between successive interactions with the sample boundary, which is proportional to the characteristic size of the sample $l_{\text{bound}} \sim l_{ch}$.

Figure 1.
Relaxation times of phonons from [8] for temperatures 300K and 30K.
Upper indexes describe normal (n) and Umklapp (u) processes.
Lower indexes correspond to longitudinal (LA) and transverse (TA) polarization.
This approach allows estimating the mean free path \( \tilde{l}_e(T) \) as a function of temperature instead of considering \( l(j, \omega, T) \):

\[
\tilde{l}_e(T) = \frac{\sum_{j} \int_{0}^{\infty} h_0 \frac{df_j(\omega, T)}{dT} D_j(\omega) \nu_{s,j}(\omega) l_j(\omega, T) d\omega}{\sum_{j} \int_{0}^{\infty} h_0 \frac{df_j(\omega, T)}{dT} D_j(\omega) \nu_{s,j}(\omega) d\omega}.
\]

Thus, for a given sample, the heat transfer regime will be determined by the characteristic sample size and temperature

\[
Kn = Kn(T, l_{ch}) = \frac{\tilde{l}_e(T)}{l_{ch}}.
\]

The results of the calculations for silicon are illustrated in figure 2.

![Figure 2](image)

**Figure 2.** Estimation of the heat transfer regime for silicon:
- \( Kn \ll 1 \) – diffusion regime;
- \( Kn \approx 1 \) – diffusion-ballistic regime;
- \( Kn \gg 1 \) – ballistic regime.

The final diagram (figure 2) is useful in practice, as it opens up ways to manage the heat transfer regime and to create structures with the necessary properties. It can be seen that the influence of boundaries occurs not only in micro- and nanoscale structures (the size effect), but also in structures with a characteristic size \( l_{ch} = 1 \) mm at temperature \( T = 50 \) K and below.

### 3. Estimating the phonon wavelength

The next characteristic size is the phonon wavelength, which can be represented in the following form:

\[
\lambda_{ph} = \frac{2\pi}{k} = \frac{2\pi}{\omega} v_{ph}(\omega).
\]

From definition (5) we can conclude that the wavelength of the phonon is a function of its frequency \( \omega \) and the phase velocity of the phonon \( v_{ph} \). In this paper the velocities \( v_{ph}(\omega) \) obtained from the polynomial approximation of experimental data are used [3].

It should be noted here that, according to the equation for thermal conductivity (1), phonons of different frequencies make different contribution to heat transfer (thermal conductivity) depending on the considered temperature. Therefore, there is a task of considering the contribution of phonons with
different wavelengths to heat transfer as a function of temperature. To do this, we use the expression (1) with a variable upper limit [9]:

$$\delta(T, \lambda) = \frac{1}{k_{\text{bulk}, j} v_{\omega j}} \int_{\omega_{\text{min}}}^{\omega_{\text{max}}} df_{\omega} \frac{D_{j}(\omega) v_{\omega j}(\omega) l_{j}(\omega, T)}{d\omega} d\omega.$$  \hspace{1cm} (6)

The results of calculation for silicon using equation (6) are shown in figure 3. For example, let's analyze the fraction of phonons that contribute ~50% in thermal conductivity (area between blue \(\lambda_1\) and yellow \(\lambda_{50}\) lines). For low temperature (about 10 K) phonons with the wave length about \(3 \cdot 10^{-8} \text{ m}\) plays the main role in thermal conductivity. When the temperature increases, the influence of low wave length phonons will rise \((\lambda_{50} \sim 3 \cdot 10^{-5} \text{ m})\). In other terms, for the temperature above 100 K the high frequency phonons play a significant role in heat transfer.

![Figure 3](image)

**Figure 3.** Dependence of the average wavelengths of phonons on temperature:
\(\lambda_{\text{min}} = \lambda_{1\%}\) and \(\lambda_{\text{max}} = \lambda_{99\%}\) — the upper limit of the wavelengths of phonons that contribute 1% and 99% to the thermal conductivity, respectively, \(\lambda_{50}\) — the value of the wavelengths that contribute 50% to the thermal conductivity, etc. Solid lines correspond to transverse waves (TA), dashed lines correspond to longitudinal polarization (LA).

4. **The effect of roughness on the mean free path of ballistic phonons**

Analysis of publications dedicated to phonon scattering at the sample boundaries has shown that the vast majority is based on the Casimir-Ziman approach \([10]\). According to this classical model \([11]\) the mean free path between successive interactions of phonons with boundary consist of two factors: the length of phonon path in diffusive limit \(l_{\text{df}}\) and the probability of specular (diffuse) reflection \(p\):

$$l_{\text{bound}} = l_{\text{df}} \frac{1 + p}{1 - p}.$$  \hspace{1cm} (7)

where value \(l_{\text{df}} = l_{\text{ch}} b_s\) contains a sample size \(l_{\text{ch}}\) (diameter for wires, thickness for films, etc.) and shape factor \(b_s\) (for plates \(b_s = 1.12\), see \([11]\)). In this case, the parameter \(p\) takes into account the
roughness of the boundary with random profile of highs (described by normal distribution) and the direction of propagation of phonons according to equation [12]

\[ p(\xi, \theta) = \exp\left( -16\pi^2 \xi^2 \cos^2 \theta \right), \]  

where \( \xi = \sigma_{rms}/\lambda_{ph} \) is the dimensionless parameter that characterizes the ratio between the root mean square roughness \( \sigma_{rms} \) and the phonon wavelength \( \lambda_{ph} \); and \( \theta \) is the angle of incidence along the normal to the surface. Depending on \( \xi \), there are two limiting cases of phonon scattering at the boundary:

1. \( \xi \gg 1 \) and \( \rho = 0 \) – purely diffusion scattering (Casimir limit),
2. \( \xi \ll 1 \) and \( \rho = 1 \) – specular scattering (reflection).

As it has been shown earlier, phonons have different frequencies and polarizations, so the problem of determining the nature of scattering at the rough boundary is multiparametric. In this regard, the specular reflection parameter is usually taken as an average and used to fit the calculation results to the experimental data, ignoring the physics of the scattering process at the boundary and the surface structure [3].

To determine the effect of temperature on the specular reflection coefficient, we analyze the dimensionless value \( \xi = \sigma_{rms}/\lambda_{ph} \). As shown in section 3, the average wavelength of phonons depends on the polarization and temperature, so

\[ \xi(j, T, \sigma_{rms}) = \frac{\sigma_{rms}}{\lambda_{ph}(j, T)}. \]  

As an example, let us consider silicon. For the average wavelength of phonons \( \bar{\lambda} \), we take the value \( \lambda_{Si} \) (the wavelengths of phonons that contribute 50% to the thermal conductivity, see figure 3). According to the relation (8), we determine the specular reflection parameter as a function of temperature and polarization using the averaging over the angle of incidence \( \theta \):

\[ \bar{p}(j, T, \sigma_{rms}) = \frac{2}{\pi} \int_0^{\pi/2} \exp \left[ -4 \left( \frac{2\pi\sigma_{rms}}{\lambda_{ph}(j, T)} \cos \theta \right) \right] d\theta. \]  

The results of calculation using model (10) are shown in figure 4. The obtained dependence \( \bar{p}(T) \) looks similar to average wave length \( \bar{\lambda}_{ph}(T) \) (figure 3): for temperature above 100 K the values of \( \bar{p}(T) \) and \( \bar{\lambda}_{ph}(T) \) show weak dependence on temperature and for low temperature the dependence is nonlinear.

Moreover, the obtained diagram is useful for explaining physics of phonon scattering. So, phonons at low temperatures have the average wave length \( \lambda_{Si} \) about 30 nm, and they will scatter mainly specularly on roughness \( \sigma_{rms} \) less than 5 nm and diffusely for \( \sigma_{rms} > 500 \text{ nm} \). With an increase in temperature above 100 K the value of \( \lambda_{Si} \) becomes 3 nm, and the scattering parameter \( \bar{p}(j, T) \ll 1 \) represents the Casimir limit (for \( \sigma_{rms} > 0.5 \text{ nm} \)), so the scattering is mainly diffuse.

The disadvantage of presented method is that the formula (10) and diagram on figure 4 don’t directly consider the influence of the sample size and its geometry. In fact, the propagation of phonons depends on allowed angles of propagation in the region between boundaries. As the geometry of the sample becomes confined, the distribution by angle \( \theta \) takes to be nonuniform. Therefore, the model (10) is useful for \( l_a > \lambda_{ph} \) or in other words for structures where phonons can exist along restriction directions.
Figure 4. Average specular reflection parameter (10) of Silicon for the mean-square roughness values: 0.1 nm, 0.5 nm, 1 nm, 5 nm, 10 nm, 50 nm and 0.5 µm. Solid lines correspond to transverse waves (TA), dashed lines represent the longitudinal polarization (LA). The numbers on figures show the values of parameter $\overline{p}$ at $T = 150$ K.

Conclusions

Based on the analysis of heat transfer in micro- and nanoscale structures, in which the heat carriers are quasi-particles phonons, it has been shown that the heat transfer regime is determined by the temperature and a set of characteristic linear dimensions: the mean-square roughness, the characteristic sample size, the average wavelength of phonons and the mean free path. Statistical model for estimating the heat transfer regime and the scattering mechanism at the boundary, depending on the value of the characteristic size of the sample and its temperature, have been formulated. As an example, calculations have been made for silicon and corresponding diagrams have been obtained for the further use in practice.

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