Discipline of “Thermal Physics of Nanostructures”

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Abstract. Thermal physics of nanostructures is an important fundamental field in the development of nanotechnology. The study of thermal processes in nanostructures requires the developing of new physical models and new mathematical tools – statistical methods of analysis of heat transfer. This work presents the subject matter of the discipline of “Thermal Physics of Nanostructures” taught at BMSTU to prepare highly qualified specialists in this new field of science and technology.

1. Introduction

Thermal physics of nanostructures is the science field studying a) thermodynamic properties and transport processes in solids with the typical size of an order less or much less than the mean free path of heat carriers in infinite medium, b) radiation heat transfer in nanogaps and c) heat transfer in nanoliquids (fluids that contains solid particles of nanometer scale) \cite{1, 2}. In the framework of this science field the samples of 3D, 2D, 1D and 0D structures are considered \cite{3, 4, 5}.

Thermal physics of nanostructures is significantly different from classical laws of thermal physics. Within this science field the laws of classical thermal physics such as Fourier law, Stefan-Boltzmann law, Newton-Richman law cannot be used, since they are applicable when mean free paths of heat carriers are much less than the size of the samples. In order to determine the areas of these two scientific directions one can use the dimensionless parameter, Knudsen number, $Kn = l/L$, where $l$ is the mean free path and $L$ is the size of sample \cite{6}. Laws of classical thermal physics are performed when $Kn \ll 1$. The area of thermal physics of nanostructures is in the range of $Kn \leq 1$. In this area two regimes of thermal transport are considered. The first is called the ballistic regime at $Kn \gg 1$ and the second is the quasi-ballistic regime, $Kn = 1$.

Heat transport in nanostructures is one of the basic science directions providing development of various nanotechnologies \cite{7}. For example, size reduction of electronic devices to nanometer scales leads to a sharp decrease of their thermal conductivity and an increase of Joule heating of all elements of the circuit. In other words, thermal resistance of the system is increased. In order to provide the required heat conditions of electronic circuits it is necessary to create reliable methods of calculation of thermal regimes in nanometer scales.

This paper presents the most important problems of development of the thermal physics of nanostructures.
2. The basics of thermal physics of nanostructures

2.1. Features of phonons
Classical thermal physics is based on phenomenological laws. In the framework of phenomenological approximation any substance is considered as continuous medium. It means that discrete atomic structure of solids, quantum properties of different fields and etc. are not taken into account. On the contrary, thermal physics of nanostructures is based on statistical physics that considers real structure of solids and thermal transport by quants of quasi-particles.

The pictures of thermal transport processes in this field are really dissimilar. Firstly, thermal carriers in metals are electrons, and in semiconductors and dielectrics these are phonons. Secondly, properties of phonons in various materials are different and require a special analysis. Third, different materials contain sets of different phonons. For example in silicon there are longitudinal and transverse phonons, and in graphene there are longitudinal, transverse and flexural phonons. The flexural phonons make a significant contribution to thermodynamic and kinetic properties.

Properties of semiconductors and dielectrics are discussed below since these materials are widely used at present. Consequently, an important part of lectures has to be devoted to phonon properties and phonon-phonon interactions.

Phonons are quanta of elastic waves that spread in solids. They are quasi-particles with zero mass. Energy of phonon is $\hbar \omega$, quasi-moment is $\hbar \vec{k}$, and velocity is $\vec{v} = \partial \omega / \partial \vec{k}$, where $\omega(k)$ is the dispersion relation. This function is determined from experiment or from the system of equations describing vibrations of solid crystal lattice in harmonic approach.

Phonon-phonon interactions depend on several factors. First of all these interactions include three phonons. Any interaction may be either a breakup of one phonon into two or a merger of two phonons into one. For silicon it is necessary to take into account the following interactions of longitudinal (LA) and traverse (TA) phonons:

\[ TA + LA \leftrightarrow LA, \quad TA + TA \leftrightarrow LA. \]

Finally two types of phonon-phonon interactions exist:
1) normal processes. As a result, N-processes save energy and total quasi–momentum:

\[ \omega_1 + \omega_2 = \omega_3, \quad \vec{k}_1 + \vec{k}_2 = \vec{k}_3. \]

2) umklapp processes. U-processes take place only at the merger of phonons at temperatures over 50 eV. As a result, energy is saved but part of quasi-momentum $\vec{G}$ passes to the lattice, $|\vec{G}| = 2\pi/a$, where $a$ is the lattice constant. In this event equations of energy and quasi-momentum conservation are written as:

\[ \omega_1 + \omega_2 = \omega_3, \quad \vec{k}_1 + \vec{k}_2 = \vec{k}_3 + \vec{G}. \]

2.2. Heat transfer in solids

2.2.1. Thermal conductivity of solids. For determining thermal conductivity in solids the equation of Boltzmann-Peierls is used. In simplest assumption of relaxation time approximation (RTA) this equation is written as:

\[ \vec{v} \cdot \nabla T \frac{\partial f}{\partial r} = f^0 - f \frac{\tau}{\tau} \]

Here $f$ is the calculated distribution function, $f^0 = \exp(\hbar \omega / k_b T) - 1$ is the equilibrium Bose-Einstein distribution function, $\vec{v}$ is the phonon velocity, $k_b$ is the Boltzmann constant, $T$ is the
temperature of solid, and $\tau$ is the relaxation time, depending on all types of phonon interactions. Relaxation time is determined by Matthiessen’s rule:

$$\frac{1}{\tau} = \frac{1}{\tau_{ph}} + \frac{1}{\tau_{r}} + \frac{1}{\tau_{b}}$$

In this formula $\tau_{ph}$ is the time between consecutive phonon-phonon interactions (phonon “life time”), $\tau_{r}$ is the time between phonon-imperfection interactions, and $\tau_{b}$ is the time between phonon–boundary interactions.

Next step is the analysis of lattice dynamics. This is very important for determining general properties of phonons. First of all it is the dispersion relations $\omega(k)$. Secondly it is phonon “life time”, $\tau_{ph}$, that is determined from the solution of vibration equations of crystal lattice in anharmonic approximation. Solution of dynamic equations in quasi harmonic approximation allows determining thermal expansion of solids. For each lattice, different equations should be solved.

For determining thermal conductivity, numerical methods, such as molecular dynamic, Monte-Carlo, etc., are widely used.

Figure 1 presents results of calculations of effective thermal conductivity of silicon films of different thickness depending on temperature [8]. Results are compared with the experimental data.

![Figure 1. Thermal conductivity of silicon films of different thickness [8]: 1 – 10 nm, 2 – 30 nm, 3 – 50 nm, 4 – 100 nm, 5 – bulk silicon, 6 – experimental data.](image)

Decreasing thermal conductivity of films is explained by the influence of phonon interactions with boundaries. It leads to a decrease of phonon mean free path while thermal conductivity is proportional to MFP. For example, thermal conductivity of bulk silicon at room temperature (300 K) is 146 $W/(m \cdot K)$, and for the film with 10 nm thickness it is 13 $W/(m \cdot K)$.

2.2.2. **Heat conductivity of monatomic structures is considered separately.** First of all, we talk about carbon structures such as graphene, carbon nanotubes, and graphene nanoribbons. Besides similar structures are silicen, phosphorens, stanen and etc.

Thermal conductivity of graphene is $3000 – 5000 W/(m \cdot K)$ at 300 K while thermal conductivity of copper is $400 W/(m \cdot K)$. It is noteworthy that for graphene, thermal expansion is negative in the range from 0 to 900K [9]. Graphene nanoribbons are very perspective for future nanoelectronic
devices. For example, it is possible to control thermal and electrical conductivity of carbon nanoribbons by changing geometrical characteristics (length, width, chirality). In figure 2 the layer of graphene is presented, the distance between nearest carbon atoms being 0.142 nm.

![Graphene](image.png)

**Figure 2.** Graphene.

2.2.3. **Contact thermal resistances (Kapitza resistances).** Heat transfer across thermal contact of dissimilar materials is a very important problem of thermal physics of nanostructures [10]. This is due to the fact that total contribution of the so called thermal boundary resistances (TBR) in general thermal resistance of nanostructures is very large. Figure 3 presents the results of numerical calculation of TBR (Kapitza resistance) and experimental data [11] for sapphire-lead interface.

![Kapitza resistance](image.png)

**Figure 3.** Kapitza resistance $R_b$ for sapphire-lead interface: theoretical value when the heat flux is from lead to sapphire (1) and from sapphire to lead (2). Experimental data for different roughness of materials [11]: $3 - Ra < 0.5 \mu m$, $4 - Ra = 4 \mu m$, $5 - Ra = 8 \mu m$.

At present there are two theories of Kapitza resistance. The first is the acoustic mismatch model (AMM) [12]. This theory is based on analysis of reflection and refraction processes of elastic waves during the transmission through the contact surface. This theory suggests specular reflection of waves. Consequently AMM is restricted by the condition that the wave length has to have more than average value of roughness of the contact surface. As a rule such condition is performed at low temperatures. The second theory is the diffusion mismatch model (DMM). This theory is based on the analysis of phonon diffusion processes during the crossing of the transition layer between two different materials. DMM can be used in all ranges of temperature and roughness.

2.3. **Heat transfer in transistors**
Especially important and complex is the analysis of thermal state in transistors [13]. The corresponding problem includes self-consistent consideration of electrical field formation within the transistor, heat generation by electrons, phonon generation by electrons, as well as electron and
phonon transport. The main difficulty of this problem is a significant non-equilibrium state of electrons in the area with strong electrical fields of the order of 50 kV/cm. It leads to non–local electron conductivity and emergence of so-called “hot spots” on the surface of transistors. In figure 4 (from article [13]) it is sown that usual drift-diffusion approximation is unsuitable for describing the processes in nanotransistors. Correct results are given by numerical method of Monte-Carlo.

![Figure 4](image-url)

**Figure 4.** Results of numerical calculations of processes within transistors [13].

a) distribution of electric potential, b) distribution of power dissipation,
d) dispersion function, c) energy of phonon generation.

3. Conclusion
The paper presents the most important features of thermal physics of nanostructures – a new field of science and technology that is being rapidly developed. It is shown that the mathematical apparatus and physical basis of this new area are fundamentally different from the classical heat transfer. Therefore to prepare new specialists with high qualification, skills and wide outlook in heat transport of nanostructures, this paper presents the discipline of “Thermal physics of nanostructures” and the basics of physical and mathematical features of this direction in details.

Acknowledgment
The work was supported by the Ministry of Science and Higher Education of the Russian Federation, project 16.8107.2017/6.7.

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