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Solid-solid thermal contact problems: current understanding

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Abstract. The past 40 years of theoretical and experimental research on contact heat transfer are reviewed. Thermophysical and mechanical processes involved in heat flow propagation through various kinds of solid-solid joints are considered. Analytical and semiempirical expressions are presented, which simulate these processes both under vacuum conditions and in the presence of a heat-conducting medium in gaps. Reasons for the experimentally examined heat flux rectification are explained. Studies on thermal contact under a nonstationary regime are covered, as is the possibility of applying classical heat conduction theory to describing the contact thermal properties. A thermodynamic interpretation of the thermal contact resistance is suggested and basic approaches to the study of contact phenomena are described. The heat conduction in nanosystems is briefly reviewed. Theoretical problems yet to be solved are pointed out and possible solution methods suggested.

1. Introduction

Analysis of the current literature on contact heat transfer in solids confirms it to be a topical subject given much attention at almost all international conferences on heat-and-mass transfer.

Since the 1970s, the problem of contact heat transfer in solids has been highlighted in this country in four monographs [1–4], two textbook chapters [5, 6], and some 80 journal papers. Over 300 works published abroad during the same

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Received 2 December 2008, revised 15 April 2009 Uspekhi Fizicheskikh Nauk **179** (9) 945–970 (2009) DOI: 10.3367/UFNr.0179.200909c.0945 Translated by Yu V Morozov; edited by A Radzig period have been cited in review articles [7–10] and in *Teplo*and Massoobmen Referativnyi Zhurnal (Heat-and-Mass Transfer Abstracts).

These publications can be arbitrarily categorized as follows:

— articles in which contact thermal conduction is regarded as a purely physical phenomenon;

— experimental studies designed to elucidate new types of joints and develop methods for detecting thermal contact resistance;

— papers in which special problems are considered, such as contact geometry, loading cycles, and attendant phenomena in the neighborhood of joints between various materials;

— applied studies aimed at introducing advanced developments into different branches of industry for reducing unproductive losses of temperature head in various construction joints, and for thermal regulation and solving the problems related to the creation of mechanically strong heat insulation with high thermal contact resistance.

Contact thermal conduction is essentially a surface effect due to the thermal and mechanical properties of interacting materials and gap-filling substances. Low thermal conductivity of a medium between loose contact surfaces accounts for the worst possible joint where contact heat transfer is largely governed by surface phenomena. The best joints are produced by welding, soldering, or vacuum deposition of one material layer over the surface of another, and their thermal contact resistance depends on the conductance of the involved materials. All other variants are intermediate between these two extremes.

2. Brief overview of theoretical and experimental studies

Over 100 studies have been concerned with the contact heat conduction theory during the past 30 years. Many of them are based on the Holm theory [11] developed for electrical contacts and extended to thermal joints. The following issues have been considered: — thermal resistance of a single microscale contact [12– 15] between a flat surface and a sphere or between a flat surface and a cone in a vacuum;

- thermal resistance of a multipoint contact in a vacuum [16, 17];

- thermal resistance of a solid-solid joint with regard for surface deformation [7, 18];

— nominally flat rough surfaces [1, 4, 7, 15];

— the effect of surface macroroughness and waviness on contact heat transfer [1, 4, 19, 20].

Also studied was the influence of surface films, interstitial defects, and chemical potential on heat exchange in intercontact gaps. Issues pertaining to numerical solution of a conjugate contact heat transfer problem in a system of solids were considered in monograph [21].

Simulation of a contact between microasperities on interacting surfaces in the form of a single joint of spherical or conical protrusions yielded no qualitatively new solutions. Only separate corrections for special cases of contact heat exchange to the well-known Royce and Yovanovich solutions were obtained [4].

The authors of Ref. [13] considered a thermal model of contact heat exchange between rough surfaces, taking into account flow curvature caused by constriction of the lines of flow to contact spots. The model was used to calculate thermal contact resistance at low pressures.

Comprehensive analysis of unitary models was reported in Ref. [22] that substantiated the necessity to consider spherical elements making contact with each other. A similar approach was taken by foreign authors [14, 17] reporting detailed studies of thermal processes in model elements.

One of the most intricate aspects of contact heat transfer is translation of unitary model solutions to real surfaces. As known from the literature, a key factor when passing to nominally flat surfaces is not only the number and size of contact spots but also the type of deformation.

Studies of large-scale surface asperities show that waviness and departure from flatness are responsible for enhanced thermal contact resistance; in addition, the influence of waviness becomes critical when there are small loads [23].

A promising approach proposed in Ref. [24] is based on the construction of random three-dimensional temperature distribution, making use of an extensive and continuously developing mathematical apparatus of the probability theory. This study demonstrated the strong influence of the anisotropic properties and mutual orientation of the surfaces on contact characteristics.

Most experimental studies were devoted to the investigation of the dependence of thermal contact resistance on the real contact area, thermal conductivity of contact pair materials, and intragap medium. The materials of interest include 1X18H9T, 12X18H10T, 45, 30, 1X13, and 30XGSA steels, copper, aluminium, D16T duralumin, Armco iron, and molybdenum treated at 300–900 K with a mechanical load of 0.1–20 MPa in the air, a vacuum, helium and argon ambient gas to obtain a roughness class in the range from 4 to 10. Some foreign authors also used materials having no analogs in the standard specifications adopted in this country.

Certain more recent studies were designed to measure the thermal conductance of contacts between advanced composite, laminated, and porous materials [25–28]. The results of an investigation into metal–semiconductor contacts were reported in monograph [29]; in particular, aluminium– silicon and semiconductor–semiconductor contacts were explored in Refs [30, 31] and [32], respectively. Values of thermal contact resistance thus obtained for carbon and carbonaceous composite materials at low temperatures [33] indicate that despite the high thermal conductivity of these materials the thermal resistance of their contacts is 100 times that in a copper–copper pair.

Adhesive-bonded joints of 12X18H10T steel specimens were subjected to a magnetic field to measure thermal conductivity of polymer glue layers with ferromagnetic filling material and to estimate the influence of an electric field on thermal conductance of polymer glue layers containing a nonferromagnetic filler [34]. It was shown that application of a magnetic or electric field to glue layers with disperse fillers during hardening allows their thermal conductivity to be increased.

Reviews [1, 2, 4, 7–9] summarize a wealth of experimental data, including the well-known correlation dependences [8, 35, 36].

Experiments designed to examine pressure effects on the thermal and electrical properties of contact junctions are reported in Ref. [37]. An acoustic study of Fe–Cu, Fe–Al, Fe–Ti, and Cu–Al contact pairs at a joint zone temperature of 310–348 K showed that the most significant changes in the real contact area A_r occur within the nominal pressure range of 12 MPa $\leq P_n \leq 40$ MPa; at $P_n > 90$ MPa, the real contact area is close to the nominal value A_n . In this process, the pressure derivative of thermal contact resistance $R_{\text{th, c}}$ tends to vanish:

$$\lim_{A_{\rm r}\to A_{\rm n}}\frac{\partial R_{\rm th,\,c}}{\partial P_{\rm n}}=0\,.$$

In fact, the quantity $R_{\text{th,c}}$ tends to a small finite value $R_{\text{th,r}}$ rather than to zero, corresponding to the thermal resistance of a real contact:

$$\lim_{A_{\rm r}\to A_{\rm n}}R_{\rm th,\,c}=R_{\rm th,\,r}>0\,.$$

This means that the solid–solid interface in a real contact zone has finite thermal conductance; in other words, thermal resistance of a close contact is nonvanishing. The contribution of real contact resistance and associated constriction resistance to the total resistance of a bimetallic system increases with decreasing resistance of the solids themselves and growing nominal pressure: it is 8–18% at $P_n = 30$ MPa, and 36–63% at $P_n = 70$ MPa; at P_n exceeding 90–100 MPa, $R_{\text{th, c}} \approx R_{\text{th, r}}$.

The authors of Ref. [37] attribute the existence of intrinsic thermal resistance in close solid–solid contacts to electron and phonon scattering at the interface between continuous media. The lack of other interpretations of such data may be due to the difficulty of applying the classical heat conduction theory at the points of discontinuity of the temperature distribution and the thermophysical properties; the theory contains the notion of fictitious contact conductance (or similar quantities) having no physical sense and hampering the understanding of the causes of experimentally examined phenomena.

3. Contact heat transfer models

The possibility of a thermoelectric analogy in a contact accounts for the similarity of the theories of contact thermal and electric conduction [38, 39]. The thermal and electrical resistance of a contact has identical components, viz. constriction resistances toward real contact spots, resistances of real contact spots and oxide films, and medium resistance in the gaps between contacts. The difference reduces to the relative values of individual components between thermal and electric conductions. The electrical resistance of oxide films is a dominant constituent of integral contact electrical resistance; an analogous component of thermal resistance is usually small compared with the total thermal contact resistance. At the same time, both thermal and electrical conductances of intercontact gaps in most gaseous media and in a vacuum are small compared with conductance of real contact spots. The structure of the thermal resistance of a real contact is determined from the equivalent scheme constructed in analogy with the electrical scheme of a given contact [40].

The main problem in the theory of solid-solid contact heat exchange consists in elucidating the relationship between the heat flux (or its density) passing through a joint and the temperature difference between the interacting surfaces. The solution to this problem requires the following main steps:

— establishment of the geometry of a system of solids under given thermomechanical conditions;

— evaluation of the influence of the geometry on temperature distribution within the confines of each continuous system;

— computation of the thermophysical properties in perturbed layers of a material for a given temperature distribution;

— calculation of the thermal contact resistance responsible for the loss of temperature head in contiguous solids as the ratio of the reduced temperature drop on mean contact planes to heat flux density:

$$R_{\rm th,\,c} = \frac{1}{\alpha_{\rm th,\,c}} = \frac{\Delta T}{q} \,, \tag{1}$$

where $\alpha_{\text{th,c}}$ is the thermal conductance of the contact, W m⁻²K⁻¹; $R_{\text{th,c}}$ is the thermal contact resistance, m² K W⁻¹; q is the heat flux density, W m⁻², and ΔT is the contact temperature drop, K. Thermal conduction problems at the solid–liquid (or gas) boundary are convenient to solve by introducing the thermal resistance of the contact [15].

Apart from $R_{\text{th,c}}$, absolute (total) thermal contact resistance $R_{\text{th,c,a}}$ is used, being defined as the ratio of contact temperature drop ΔT to heat flux Q [41]:

$$R_{\rm th,\,c,\,a} = \frac{\Delta T}{Q} \,. \tag{2}$$

Unlike thermal contact resistance, absolute thermal resistance $R_{\text{th,c,a}}$ corresponds to the entire surface across which the heat flux is transferred rather than to a unit area of the heat exchange surface.

The parameters of surface roughness and waviness, as well as the mechanical characteristics of a contact, are identical for thermal and electric conductions. In heat exchange between a solid and a gas (or a liquid), the solid surface structure largely affects the convective constituent. Thermal conductivity of solid–gas or solid–liquid interfaces, such as occurring, in particular, in intercontact gaps during heat transfer in solids, depends first and foremost on the thermodynamic and thermophysical properties of the interacting systems and on the pressure of the medium (gas or liquid) in which the contact takes place. The situation with thermal conductivity in solid-solid contacts is different. Surface and mechanical properties of the solid-solid interface determine the real contact area which in turn accounts for the value of constriction resistance. Heat flow density increases near real contact zones (i.e., flow lines contract in these zones), similar to electric current density in such zones (constriction of electric current lines to the real contact zones) in the case of electric conduction when this constituent of contact resistance results from a decrease in the flow area for electrons from the nominal cross section area of the body to the real contact area. However, electrical constriction resistance has a clear physical interpretation due to the constriction of electric current lines to real contact zones along the electron flow trajectory, while thermal constriction resistance is explained purely phenomenologically. In a homogeneous medium with a steady-state temperature, a heat flow line is a curve constructed in such a way that the constant temperature gradient vector directed from one isothermal surface to another is always oriented tangentially to this line (Fig. 1). Solid-solid thermal contact is associated with distortion of isothermal surfaces. As a result, heat flow lines turn out to be contracted to the zones of intimate joint of surfaces [42]; in other words, energy transfer by thermal conduction unlike that by electrical conduction, occurs without matter transfer.

Due to the waviness and roughness of a solid surface, heat flow constriction occurs in a step-by-step mode: first, flow lines contract to contact macrospots formed by waviness within nominal cross sections and thereafter to roughnessproduced microspots within the confines of each macrospot (Fig. 2) [40]. Under real conditions, mechanical interaction between surfaces takes place only at contact microspots, while macrospots are just regions where microspots concentrate. The distance between real contact spots increases with decreasing contact pressure, and the microspots become thermally equivalent to single contacts modelled as the bases of semi-infinite cylinders (tubes of heat flow) [43]. Such an approximation allows the multidimensional thermal conduc-



Figure 1. Constriction of heat flow lines to real contact zones.



Figure 2. The structure of constriction resistance.

tivity problem to be reduced to a unidimensional one, thereby simplifying calculations. The arithmetic average of radii $a_1, a_2, \ldots, a_{n_r}$ gives the mean equivalent radius *a* of the contact spot:

$$a=\frac{1}{n_{\rm r}}\sum_{i=1}^{n_{\rm r}}a_i\,,$$

where n_r is the number of real contact spots [44]. Contact spot itemized under number *i* has its own temperature $T_{c,r,i}$. These temperatures and corresponding radii a_i are responsible for the establishment of temperature distribution in the contact area for which mean contact temperature $\overline{T}_{c,r}$ is given by [45]

$$\bar{T}_{\rm c,r} = \frac{\sum_{i=1}^{n_{\rm r}} a_i T_{\rm c,r,i}}{\sum_{i=1}^{n_{\rm r}} a_i} \,.$$

Therefore, the temperature drop in contact, $\bar{T}'_{w,2} - \bar{T}''_{w,2}$, may be expanded into two parts (Fig. 3):

$$T'_{\rm w,2} - T''_{\rm w,2} = (T'_{\rm w,2} - \bar{T}_{\rm c,r}) + (\bar{T}_{\rm c,r} - T''_{\rm w,2}) \,.$$

If heat flux vectors crossing real contact spots are parallel, i.e., in the case of a unidimensional problem, the terms on the right-hand side of the last equation can be represented as [45]

$$T'_{\rm w,2} - \bar{T}_{\rm c,r} = \frac{\delta_1 q}{\lambda_1} , \quad \bar{T}_{\rm c,r} - T''_{\rm w,2} = \frac{\delta_2 q}{\lambda_2} ,$$

where q is the heat flux density across the contact plane, W m⁻²; λ_1 , λ_2 are the thermal conductivities of interacting solids, and δ_1 , δ_2 are the functions characterizing the constriction of heat flow lines to real contact spots in materials 1 and 2, m. These functions are identical because they depend on microgeometry alone (the distribution of contact zone radii $a_1, a_2, \ldots, a_{n_r}$ within contact contour area F_a), which is identical for the two materials, and on the thermal conductance of contacting media; hence follows the relationship

$$\frac{T'_{\rm w,2} - \bar{T}_{\rm c,r}}{\bar{T}_{\rm c,r} - T''_{\rm w,2}} = \frac{\lambda_2}{\lambda_1} ,$$

from which the mean contact temperature can be found:

$$\bar{T}_{c,r} = \frac{T'_{w,2} + (\lambda_2/\lambda_1) T''_{w,2}}{1 + \lambda_2/\lambda_1} \,. \tag{3}$$



Figure 3. Temperature distribution in a solid–solid contact (thermal conductivity increases with temperature in solid 1, and decreases in solid 2).

Whether the contact is elastic or plastic depends on the value of $\overline{T}_{c,r}$. In other words, $\overline{T}_{c,r}$ determines real contact pressure P_r and thereby real contact area A_r :

$$A_{\rm r} = \frac{N}{P_{\rm r}}$$

where N is the compressive force, N, directed to the contact surface.

The ratio of the real-to-nominal contact areas describes constriction resistance that, in many cases of practical significance, exceeds other constituents of thermal contact resistance:

$$R_{\mathrm{th,\,cn}} = \frac{1}{\alpha_{\mathrm{th,\,cn}}} \sim \frac{A_{\mathrm{r}}}{A_{\mathrm{n}}} \, .$$

These other components of contact thermal conductance $\alpha_{th, c}$ include:

- medium conductance in intercontact gaps, $\alpha_{th,m}$;
- surface film conductance, $\alpha_{th, f}$;
- conductance during radiative heat transfer, $\alpha_{th, rad}$ [6];

— conductance during heat transfer by emission and electron tunneling across the contact zone, $\alpha_{th, em}$, $\alpha_{th, tun}$ [38, 46].

Real contact conductance $\alpha_{th,r}$ deserves to be considered separately for the following reason. A real contact tightly binds solid surfaces together, being close to ideal joint; therefore, thermal resistance $R_{th,r}$ of the real contact is very low and the temperature during passage through the contact spots is assumed to be continuous. However, constriction resistance $R_{th,cn}$ related to the contact spot area is rather high. Not infrequently, real contact resistance is associated with constriction resistance directly related to the real contact zone. Construction of an equivalent scheme is one of the most accurate methods for calculation of thermal contact resistance (or corresponding conductance). Because areas crossed by heat fluxes corresponding to one component of total resistance or another differ [e.g., the active areas of tunneling $(R_{th,tun})$ and emission $(R_{th,em})$ constituents of thermal contact resistance are equal to nominal A_n , while the active area of constriction resistance $R_{th,en}$ is identical to real A_r], the equivalent scheme in the general form is applicable to specific (1) and absolute (2) thermal resistances expressed as the ratio of specific quantities to the corresponding active areas:

$$\begin{split} R_{\rm th, c, a} &= \frac{R_{\rm th, f, 1} + R_{\rm th, f, 2}}{A_{\rm n}} \\ &+ \left[A_{\rm n} \left(\frac{1}{R_{\rm th, tun}} + \frac{1}{R_{\rm th, em}} \right) \right. \\ &+ \left(A_{\rm n} - A_{\rm r} \right) \left(\frac{1}{R_{\rm th, m}} + \frac{1}{R_{\rm th, rad}} \right) + \frac{A_{\rm r}}{R_{\rm th, cn, 1} + R_{\rm th, cn, 2}} \right]^{-1}, \end{split}$$

where $R_{\text{th, tun}}$ is the thermal resistance in electron tunneling; $R_{\text{th, em}}$ is the resistance in electron emission; $R_{\text{th, rad}}$ is the resistance in radiative heat exchange in a contact; $R_{\text{th, m}}$ is the resistance of the medium in intercontact gaps; $R_{\text{th, cn, 1}}$, $R_{\text{th, cn, 2}}$ are the constriction resistances in materials 1 and 2, and $R_{\text{th, f, 1}}$, $R_{\text{th, f, 2}}$ are the film resistances at interacting surfaces of materials 1 and 2, m² K W⁻¹. Nevertheless, given the equality of active areas of individual constituents (e.g., constriction resistance $R_{\text{th, cn}}$ and real contact resistance $R_{\text{th, r}}$), the equivalent scheme can be just as well constructed for their specific resistances.

Such an approach requires detailed consideration of each component and an adequate method for its detection. The following assumptions are feasible depending on the statements of the problem:

— thermal resistance of the films is close to zero, $R_{\text{th, f}} \rightarrow 0$, due to their small thickness [47];

— at mean contact temperature $\bar{T}_{c,r}$ below 700–1000 K, heat transferred by radiation does not exceed 2–3% of the total thermal flux; at moderate temperatures, radiative heat exchange in the first approximation may be neglected, i.e., $\alpha_{th, rad} \rightarrow 0$ [6, 48, 49];

— if mean contact temperature $\bar{T}_{c,r}$ does not exceed 2000 K and film thickness δ_r is above 1 nm, the energies transferred through the contact interface by electron emission and tunneling are small compared with phonon heat transfer and $\alpha_{th,em} \rightarrow 0$, $\alpha_{th,tun} \rightarrow 0$ [45, 50];

— thermal resistance of a real contact sequentially introduced at each interface is close to ideal one, $R_{\text{th, r}} \rightarrow 0 = R_{\text{th, i}}$; therefore, it is excluded from the equivalent scheme as a low-value series component.

Thus, thermal resistance $R_{\text{th, c, a}}$ of a real contact can be expressed through thermal constriction resistances $R_{\text{th, cn, 1}}$, $R_{\text{th, cn, 2}}$ in the first and second materials and through thermal resistance of the medium in intercontact gaps, $R_{\text{th, m}}$ (Fig. 4):

$$R_{\rm th, c, a} = \frac{1}{(A_{\rm n} - A_{\rm r})/R_{\rm th, m} + A_{\rm r}/(R_{\rm th, cn, 1} + R_{\rm th, cn, 2})}$$

where total constriction resistance $R_{\text{th,cn}}$ is the sum of constriction resistances in materials 1 and 2, namely

$$R_{\rm th,\,cn} = R_{\rm th,\,cn,1} + R_{\rm th,\,cn,2} \,.$$



Figure 4. The structure of contact thermal resistance.

If the intercontact gaps contain a vacuum, resistance of the medium is infinitely high and thermal conductance $\alpha_{th,m}$ through the gaps represented by the first term in the denominator vanishes. In this case, thermal resistance of a real contact is completely defined by the constriction resistance:

$$R_{\mathrm{th,c}} = R_{\mathrm{th,cn}}$$
.

Such a situation is common in space engineering where the equipment is operated in a vacuum, and surface films grow slowly, having no appreciable effect on contact conductance. For this reason, the primary objective of research in this field is to elucidate the mechanisms underlying the formation of constriction resistances and to develop methods for their computation.

Theoretical studies on contacts between different types of metals are divided into four main subgroups [51]:

— 'electric' ones using the electrical theory of solids for the description of thermal conduction between metallic surfaces;

— 'microscopic' ones investigating the dependence of thermal contact resistance on surface roughness;

— 'macroscopic' ones based on the boundary effect in interactions of macroscopic contact areas;

— 'film' research designed to study the influence of surface films on contact thermal conductance.

In addition, there are computation techniques combining the methods of two or more of the above subgroups. As a rule, combined methods employ basal parameters, each having some effect or another on contact heat transfer [51]. Such computation takes into account:

- waviness characteristics of the surface;
- roughness characteristics of the surface;
- mean angles of microasperities on contiguous surfaces;
- number, size, and shape of microasperities;
- contact pressure;

— loading history of materials in each experimental series, including their deformation;

— surface temperatures of the contact;

- mechanical and thermophysical properties of the materials;

— heat flux magnitude and direction;

— history of thermal loading in each experimental series, with special reference to the number of changes in the heat flux direction. One of the most popular analytical models is the following representation of constriction resistances [52]:

$$R_{\rm th,\,cn,\,a} = \frac{\psi}{2\pi n_{\rm r}\lambda a} \arctan\left(\frac{r}{a} - 1\right),\tag{4}$$

where $R_{\text{th, cn, a}}$ is the absolute thermal constriction resistance, K W⁻¹; *r* is the mean fictitious radius of the constriction area, m, and ψ is the shape factor of the contact spots, equaling 1 for circular spots. Bearing in mind that the active area of constriction resistance is the real area A_r , the following relationship is valid for specific thermal contact resistance:

$$R_{\rm th,\,cn} = \frac{A_{\rm r}}{2\pi n_{\rm r}\lambda a} \arctan\left(\frac{r}{a} - 1\right) = \frac{a}{2\lambda} \arctan\left(\frac{r}{a} - 1\right).$$
(5)

Quantities *a*, *r* are found as follows:

— by calculating thermal microconstriction resistance resulting from the constriction of heat flow lines to a single spot from radius r to a:

$$a = \sqrt{\frac{A_{\rm r}}{\pi n_{\rm r}}}, \quad r = \sqrt{\frac{A_{\rm n}}{\pi n_{\rm r}}};$$
 (6)

— by calculating the total thermal contact resistance:

$$a = \sqrt{\frac{A_{\rm r}}{\pi}}, \quad r = \sqrt{\frac{A_{\rm n}}{\pi}}.$$
 (7)

Relations (6), (7) establish the following limits for constriction resistances:

— for the specific value

$$\lim_{\substack{a \to 0 \\ A_r \to 0 \\ n_r \to 0}} R_{\text{th, cn}} = \lim_{\substack{a \to 0 \\ A_r \to 0 \\ n_r \to 0}} \frac{a}{2\lambda} \arctan\left(\frac{r}{a} - 1\right) = \lim_{\substack{a \to 0 \\ A_r \to 0 \\ n_r \to 0}} \frac{\pi a}{4\lambda} = 0$$
$$\lim_{\substack{a \to r \\ A_r \to A_n \\ n_r \to 1}} R_{\text{th, cn}} = \lim_{\substack{a \to r \\ A_r \to A_n \\ n_r \to 1}} \frac{a}{2\lambda} \arctan\left(\frac{r}{a} - 1\right) = 0;$$

— for the absolute value

$$\lim_{\substack{a\to0\\A_r\to0\\n_r\to0}} R_{\text{th, cn, a}} = \lim_{\substack{a\to0\\A_r\to0\\n_r\to0}} \frac{1}{2\pi n_r \lambda_c a} \arctan\left(\frac{r}{a}-1\right)$$
$$= \lim_{\substack{a\to0\\A_r\to0\\A_r\to0\\n_r\to0}} \frac{1}{4n_r \lambda_c a} = \infty ,$$

$$\lim_{a \to r \atop a_{\tau} \to -1} R_{\text{th}, \text{cn}, a} = \lim_{a \to r \atop a_{\tau} \to -1} \frac{1}{2\pi n_{\tau} \lambda_{c} a} \arctan\left(\frac{r}{a} - 1\right) = 0.$$

Because practically any material manufactured or processed in the air is coated with a surface film, the contact zone is chemically inhomogeneous. For this reason, the equivalent scheme should contain film resistance in a series with the resistances of the contact materials themselves (see Fig. 4):

$$R_{\text{th},c} = (R_{\text{th},f,1} + R_{\text{th},f,2}) + (R_{\text{th},cn,1} + R_{\text{th},cn,2})$$

= $R_{\text{th},f} + R_{\text{th},cn}$,

where the thermal resistances $R_{\text{th},f,1}$, $R_{\text{th},f,2}$ of the films are defined by the ratio of their mean thicknesses $\delta_{f,1}$, $\delta_{f,2}$ to their

thermal conductivities $\lambda_{f,1}, \lambda_{f,2}$:

$$R_{\text{th}, \text{f}, 1} = \frac{\delta_{\text{f}, 1}}{\lambda_{\text{f}, 1}}, \quad R_{\text{th}, \text{f}, 2} = \frac{\delta_{\text{f}, 2}}{\lambda_{\text{f}, 2}}.$$

Mean film thickness can be determined by measuring the electrical resistance of the contact [50].

If an especially high accuracy of thermal computation is needed, the scheme in Fig. 4 is supplemented by resistances of intimate contacts at each interface between the two materials. However, the low values of these resistances make relevant experiments difficult to conduct, and only a few methods for their theoretical evaluation have thus far been described in the literature [53]. Thermal resistance of an intimate contact may be defined as

$$R_{\text{th}, i, 12} = \frac{1}{2} \left(\frac{\delta_1 T + \delta_2 T}{q} \right)$$
$$= \frac{1}{2N_A^{1/3}} \left[\frac{1}{\lambda_1} \left(\frac{M_1}{\rho_1} \right)^{1/3} + \frac{1}{\lambda_2} \left(\frac{M_2}{\rho_2} \right)^{1/3} \right], \quad (8)$$

where N_A is the Avogadro constant, mol⁻¹; M_1 , M_2 are the molar masses, kg mol⁻¹; λ_1 , λ_2 are the thermal conductivities, W (m K)⁻¹, and ρ_1 , ρ_2 are the densities of materials 1 and 2, kg m⁻³.

Because the thermal resistance of an intimate contact $(\sim 10^{-11} \text{ m}^2 \text{ K W}^{-1})$ is a few orders of magnitude lower than the constriction resistance $(\sim 10^{-4} \text{ m}^2 \text{ K W}^{-1})$, it is the constriction effect that determines contact thermal conductance in the absence of a substance in the gaps. Thermal constriction resistance can be represented by the product of the ratio of perturbed zone thickness δ_{cn} to thermal conductivity λ and function Φ dependent on the real-to-nominal area ratio [54]:

$$R_{\rm th,\,cn} = \frac{\delta_{\rm cn}}{\lambda} \Phi = \frac{\delta x N_{\rm cn}}{\lambda} \cot\left(\frac{\pi}{2} \frac{A_{\rm r}}{A_{\rm n}}\right)$$
$$= \frac{1}{N_{\rm A}^{1/3}} \frac{1}{\lambda} \left(\frac{M}{\rho}\right)^{1/3} N_{\rm cn} \cot\left(\frac{\pi}{2} \frac{A_{\rm r}}{A_{\rm n}}\right), \tag{9}$$

where $N_{\rm cn} \approx 0.5 \times 10^7$ is the number of molecular layers in the perturbed zone, varying with the material, and δx is the minimal discrete change of the coordinate equaling the atomic layer thickness. Then, one finds

$$R_{\rm tn, c, 12} = R_{\rm th, r, 12} + \frac{1}{N_{\rm A}^{1/3}} \frac{1}{\lambda_1} \left(\frac{M_1}{\rho_1}\right)^{1/3} N_{\rm cn} \cot\left(\frac{\pi}{2} \frac{A_{\rm r}}{A_{\rm n}}\right)$$
$$+ \frac{1}{N_{\rm A}^{1/3}} \frac{1}{\lambda_2} \left(\frac{M_2}{\rho_2}\right)^{1/3} N_{\rm cn} \cot\left(\frac{\pi}{2} \frac{A_{\rm r}}{A_{\rm n}}\right)$$
$$= R_{\rm th, r, 12} + R_{\rm th, cn, 1} + R_{\rm th, cn, 2} = R_{\rm th, r, 12} + R_{\rm th, cn, 12} . (10)$$

The constriction effect is apparent in perturbation zones where average temperatures are close to mean contact temperature $\overline{T}_{c,r,12}$; therefore, the thermal conductivities and densities of materials in the first approximation are taken at this temperature and have the sense of the thermophysical properties of perturbation zones:

$$\lambda_1 = \lambda_1(\bar{T}_{\mathrm{c},\mathrm{r},12}), \quad \lambda_2 = \lambda_2(\bar{T}_{\mathrm{c},\mathrm{r},12})$$



Figure 5. Thickness of the perturbed zone depending on the real contact area for different nominal area values: $A_{n1} = 10^{-5} \text{ m}^2$, $A_{n2} = 5 \times 10^{-5} \text{ m}^2$, and $A_{n3} = 10^{-4} \text{ m}^2$.

According to formula (9), thermal constriction resistances has the following limits:

- for the specific value

$$\lim_{\substack{a \to 0 \\ A_{r} \to 0 \\ n_{r} \to 0}} R_{\text{th}, \text{cn}} = \lim_{\substack{a \to 0 \\ A_{r} \to 0 \\ n_{r} \to 0}} \frac{\delta x N_{\text{cn}}}{\lambda} \cot\left(\frac{\pi}{2} \frac{A_{\text{r}}}{A_{\text{n}}}\right) = \infty ,$$

$$\lim_{\substack{a \to r \\ A_{r} \to A_{n} \\ n_{r} \to 1}} R_{\text{th}, \text{cn}} = \lim_{\substack{a \to r \\ A_{r} \to A_{n} \\ n_{r} \to 1}} \frac{\delta x N_{\text{cn}}}{\lambda} \cot\left(\frac{\pi}{2} \frac{A_{\text{r}}}{A_{n}}\right) = 0 ;$$

— for the absolute value

$$\lim_{\substack{a \to 0 \\ A_r \to 0}} R_{\text{th, cn, a}} = \lim_{\substack{a \to 0 \\ A_r \to 0 \\ n_r \to 0}} \frac{\delta x N_{\text{cn}}}{A_r \lambda} \cot\left(\frac{\pi}{2} \frac{A_r}{A_n}\right) = \infty,$$
$$\lim_{\substack{a \to r \\ A_r \to A_n \\ n_r \to 0}} R_{\text{th, cn, a}} = \lim_{\substack{a \to r \\ A_r \to A_n \\ n_r \to 1}} \frac{\delta x N_{\text{cn}}}{A_r \lambda} \cot\left(\frac{\pi}{2} \frac{A_r}{A_n}\right) = 0.$$

In formula (9), the thickness of the perturbed zone is assumed to be constant, whereas another approach is realized in formula (5) where the constriction function is not used and $R_{\rm th,\,cn}$ is defined as a quantity directly proportional to the thickness $\delta_{\rm cn}$ of the perturbed zone. In this case, the thickness of the perturbed zone (hence, thermal constriction resistance) depends on the relationship between the real and nominal areas and has an extremum at $A_{\rm r}/A_{\rm n} \approx 0.201$ (Fig. 5). Therefore, a decrease in the real area in the low contact pressure range must lead to a fall of constriction resistances, and its zero value must correspond to a zero value of $R_{\text{th, cn.}}$. In both approaches, absolute constriction resistances $R_{\text{th, cn, a}}$ tend to infinity as the real contact area in the low-pressure range decreases, and they agree fairly well with experimental data for medium and high pressures. The fundamental problem of the extremum in the perturbation zone needs verification by experiment because the above methods yield different limits of constriction resistances in the low-pressure range (Figs 5, 6).

A third approach that ensures both infinitely high specific constriction resistances for a zero real contact area and extremum of the thickness of the perturbed zone in the low contact pressure range is also conceivable. This approach combines the advantages of the two above methods using the definition of the thickness of the perturbation zone from formula (5) and constriction function (9) (Φ may have a different value):

$$R_{\rm th,\,cn} = \frac{\delta_{\rm cn}}{\lambda} \Phi = \frac{a}{2\lambda} \arctan\left(\frac{r}{a} - 1\right) \cot\left(\frac{\pi}{2} \frac{A_{\rm r}}{A_{\rm n}}\right)$$
$$= \frac{1}{2\lambda} \sqrt{\frac{A_{\rm r}}{\pi}} \arctan\left(\sqrt{\frac{A_{\rm n}}{A_{\rm r}}} - 1\right) \cot\left(\frac{\pi}{2} \frac{A_{\rm r}}{A_{\rm n}}\right). \quad (11)$$

It leads to the following limits: — for the specific value

$$\lim_{\substack{a \to 0 \\ A_{r} \to 0 \\ n_{r} \to 0}} R_{\text{th, cn}} = \lim_{\substack{a \to 0 \\ A_{r} \to 0 \\ n_{r} \to 0}} \frac{a}{2\lambda} \arctan\left(\frac{r}{a} - 1\right) \cot\left(\frac{\pi}{2} \frac{a^{2}}{r^{2}}\right)$$
$$= \lim_{\substack{a \to 0 \\ A_{r} \to 0 \\ n_{r} \to 0}} \frac{\pi a}{4\lambda} \frac{\cos\left[\pi a^{2}/(2r^{2})\right]}{\sin\left[\pi a^{2}/(2r^{2})\right]} = \frac{1}{2\lambda} \lim_{\substack{a \to 0 \\ A_{r} \to 0 \\ n_{r} \to 0}} \frac{r^{2}}{a} = \infty,$$
$$\lim_{\substack{a \to r \\ A_{r} \to A_{n} \\ n_{r} \to 1}} R_{\text{th, cn}} = \lim_{\substack{a \to r \\ A_{r} \to A_{n} \\ n_{r} \to 1}} \frac{a}{2\lambda} \arctan\left(\frac{r}{a} - 1\right) \cot\left(\frac{\pi}{2} \frac{a^{2}}{r^{2}}\right) = 0;$$

for the absolute value

$$\lim_{\substack{a \to 0 \\ A_r \to 0 \\ n_r \to 0}} R_{\text{th, cn, a}} = \lim_{\substack{a \to 0 \\ A_r \to 0 \\ n_r \to 0}} \frac{1}{2\pi n_r \lambda a} \arctan\left(\frac{r}{a} - 1\right) \times \cot\left(\frac{\pi}{2} \frac{a^2}{r^2}\right) = \infty,$$



Figure 6. Experimental and theoretical values of contact thermal resistances (plastic contact): (a) for a Cu–Al contact pair at a mean contact temperature of 333 K, and (b) for an Fe–Al contact pair at a mean contact temperature of 348 K.

Despite the advantages of analytical methods for determining the thermal resistance of real contacts due to the possibility of the physically sound computation of its value, the necessity to calculate a large number of various parameters precludes fast estimation for practical purposes. This accounts for the extensive use of semiempirical dependences in calculations of contact heat exchange to evaluate integral thermal contact resistance without insight into the peculiarities of its structure.

One such method permits calculating heat exchange in contacts between different types of metals taking account of microscopic and macroscopic parameters. Total contact conductance $\alpha_{th,c}$ is represented as the sum of thermal conductances through contact spots in solids, $\alpha_{th,cn}$, and medium in the intercontact gaps, $\alpha_{th,m}$,

$$\alpha_{\rm th,\,c} = \alpha_{\rm th,\,cn} + \alpha_{\rm th,\,m}\,.$$

Terms on the right-hand side of this relation are obtained from the following empirical dependences [31, 48, 49, 55]:

$$\alpha_{\rm th,\,cn} = \eta_1 \lambda_{\rm c} \left(\frac{P_{\rm n}}{H}\right)^{\eta_2} \left(\frac{m}{\sigma}\right)^{\eta_3},$$

$$\eta_1 = 1.25, \ \eta_2 = 0.95, \ \eta_3 = 1.00 \ [31, 55], \qquad (12)$$

$$\eta_1 = \frac{2}{\pi} - \frac{2}$$

$$\begin{split} \eta_1 &= \frac{-}{\pi \chi} , \ \chi = 0.36, \ \eta_2 = 1 + 0.071 c_2, \ \eta_3 = 1.00 \ [48, 49] \\ \alpha_{\text{th}, \text{m}} &= \frac{\lambda_{\text{m}}}{\varDelta + \varGamma} , \end{split}$$

where P_n is the nominal contact pressure, Pa; $\lambda_c = 2\lambda_1\lambda_2/(\lambda_1 + \lambda_2)$ is the geometric mean of thermal conductivities of interacting materials, W (m K)⁻¹; λ_m is the thermal conductivity of the gap medium, W (m K)⁻¹; $\sigma = (\sigma_1^2 + \sigma_2^2)^{1/2}$ is the reduced surface roughness, m, and $m = (m_1^2 + m_2^2)^{1/2}$ is the mean reduced microasperity angle. Distance Δ [m] between mean planes of the contacting surfaces is given by the expression

$$\Delta = 1.53 \left(\frac{P_{\rm n}}{H}\right)^{-0.097} \sigma \,.$$

Gas parameter Γ is defined by the product of reduced accommodation coefficient α , parameter β , and mean free path Λ of a molecule in the gaps:

$$\begin{split} \Gamma &= \alpha \beta \Lambda, \quad \alpha = \frac{2 - \alpha_1}{\alpha_1} + \frac{2 - \alpha_2}{\alpha_2} ,\\ \beta &= \frac{2\gamma}{\Pr\left(\gamma + 1\right)} , \quad \Lambda = \Lambda_0 \, \frac{P_0}{P} \, \frac{T}{T_0} , \end{split}$$

where α_1 , α_2 are the accommodation coefficients at the interfaces between solid surfaces and the gap medium; *T* is the gap medium temperature, K; P_0 is the medium pressure in the gaps at room temperature T_0 , Pa; Pr is the Prandtl criterion for the medium in the gaps, and γ is the level of heat (statistical coefficient).

Surface microhardness *H* is in great excess of the Brinell value and depends on a number of parameters, such as average surface roughness σ , the mean absolute angle of material roughness $m \approx \tan m \sim 0.01-0.1$ (tilt angle of the microroughness cone generatrix), surface treatment procedure, applied pressure, and contact temperature. Surface microhardness *H* is computed with respect to nominal contact pressure P_n [48, 49]:

$$\frac{P_{\mathrm{n}}}{H} = \left(\frac{P_{\mathrm{n}}}{H'}\right)^{1/1+0.071c_2}, \quad H' = c_1 \left(\frac{1.62\sigma}{m\sigma_0}\right),$$

where $\sigma_0 = 10^{-6}$ m; c_1 , c_2 are the Vickers microhardness coefficients:

$$c_{1} = H_{\text{BGM}}(4.0 - 5.77k + 4.0k^{2} - 0.61k^{3}),$$

$$c_{2} = -0.57 + \left(\frac{1}{1.22}\right)k - \left(\frac{1}{2.42}\right)k^{2} + \left(\frac{1}{16.58}\right)k^{3},$$

$$k = \frac{H_{\text{B}}}{H_{\text{BGM}}},$$

 $H_{\rm BGM} = 3.178 \times 10^9$ Pa, and $H_{\rm B}$ is the Brinell microhardness, Pa. This approximation is valid in the hardness range of $1.3 \times 10^9 \le H_{\rm B} \le 7.6 \times 10^9$ Pa. With the fictitious value of surface microhardness $H_{\rm c}$ being known, coefficients of microhardness can be found as $c_1 = H_{\rm c}$, and $c_2 = 0$.

Thermal conductance of a real contact with regard for constriction resistances is also calculated using the semiempirical dependence [6, 32, 35] derived from generalization of numerous experimental data and yielding fairly reliable values for a variety of materials:

$$\alpha_{\rm th,s} = 1.15 \times 10^4 \lambda_{\rm eq} \left(\frac{P_{\rm n}^2}{\Omega_{\rm b} E} \, \frac{T_{\rm c}}{T_{\rm melt}} \, K^2 \right)^{0.302},\tag{13}$$
$$\lambda_{\rm eq} = \frac{\sigma_1 + \sigma_2}{\sigma_1 / \lambda_1 + \sigma_2 / \lambda_2} \,,$$

where λ_{eq} is the equivalent thermal conductivity of the contacting materials, W (m K)⁻¹; h_1 , h_2 are the mean heights of microasperities at the interacting surfaces, m; P_n is the nominal contact pressure, Pa; Ω_b is the ultimate strength of a softer material, Pa; E is the coefficient of elasticity of the contacting materials, Pa; T_c is the mean contact temperature, K; T_{melt} is the melting temperature of a lower-melting material, K; $E = 2E_1E_2/(E_1 + E_2)$ is the reduced elastic modulus, Pa, E_1 , E_2 are the reduced elastic moduli of contacting materials, Pa, and K is a coefficient describing a change of contiguous surfaces depending on the arithmetic mean of profile deflection in the following way:

$$K = 1 \text{ at } (\sigma_1 + \sigma_2) > 3 \times 10^{-5} \text{ m},$$

$$K^2 = \left(\frac{30 \times 10^{-6}}{\sigma_1 + \sigma_2}\right)^{2/3} \text{ for } 10^{-5} < \sigma_1 + \sigma_2 \le 3 \times 10^{-5} \text{ m},$$

$$K = \frac{15 \times 10^{-6}}{\sigma_1 + \sigma_2} \text{ for } \sigma_1 + \sigma_2 \le 10^{-5} \text{ m}.$$

The results of a comparison of thermal contact resistances calculated from formula (13) and found through experiment for several flat specimens in a vacuum [35] are presented in Table 1. At a confidence level of 0.95, the calculation error for thermal resistance of a contact does not exceed 52%. The difference between theoretical and observed values is due to the errors in the experimental determination of $R_{th,c}$, as well

Contact	Surface geometry						Theoretical	Experimental	
pair	R_{a1}	R _{a2}	R_1	R_2	а	ψ	λ _{eq}	$R_{ m th,c}$	$R_{\rm th,c}$
	10 ⁻⁶ m					$W(m K)^{-1}$	10 ⁻⁴ n	$n^2 K W^{-1}$	
X18H8T-X18H9T	1.15	0.68	47	180	6.2	0.989	21.1	20.5	23.1
X18H8T-X18H9T	0.46	0.40	510	718	9.4	0.982	21.1	13.1	18.4
X18H8T-X18H9T	0.38	0.42	890	628	12.0	0.968	21.1	12.4	14.0
Mo-X18H9T	0.48	0.40	580	736	9.8	0.986	42.0	37.4	25.3
X18H9T-Cu	0.52	1.26	148	43	14.0	0.972	64.3	3.38	4.8

Table 1. Measured values of contact thermal resistance at $P_n = 5 \times 10^5$ Pa, and $T_c = 550$ K.

as in the measurement of geometric characteristics, and to the assumptions adopted when using analytical relations. Specifically, the fictitious quantity necessary to account for discontinuity of thermal conduction in the contact zone is present in both formulas (12) and (13) (reduced thermal conductivity λ_c of materials in formula (12) and equivalent thermal conductivity λ_{eq} in formula (13)).

Figures 7, 8 illustrate the results of calculations of thermal contact resistances for plastic and elastic Al–Al joints in a vacuum with similar classes of finish of the interacting surfaces. Thermal resistance of a contact was found as the sum of constriction resistances in the samples (thermal resistance of the real contact was disregarded in view of its smallness). Mechanical properties and contact criterion (plastic or elastic) were obtained as described in Ref. [44]. Real pressure in the plastic contact was 1.082×10^8 Pa (Fig. 7), and in the elastic one 1.050×10^8 Pa (Fig. 8). In other words, for all the apparent similarity between Figs 7 and 8, the abscissa axis in the latter is more extended than in the former.

The above relations were converted to one and the same argument, namely

$$\frac{A_{\rm r}}{A_{\rm n}} = \frac{P_{\rm n}}{P_{\rm r}} \,,$$

as follows:

— the real contact area was expressed through the nominal one (constant for a given joint):

$$A_{\rm r} = \left(\frac{A_{\rm r}}{A_{\rm n}}\right) A_{\rm n} = \left(\frac{P_{\rm n}}{P_{\rm r}}\right) A_{\rm n}, \quad A_{\rm n} = {\rm const};$$

— the nominal contact pressure was expressed through the real one (constant for a given joint):

$$P_{\rm n} = \left(\frac{P_{\rm n}}{P_{\rm r}}\right) P_{\rm r} = \left(\frac{A_{\rm r}}{A_{\rm n}}\right) P_{\rm r}, \quad P_{\rm r} = {\rm const.}$$

The nominal contact area A_n is the starting parameter characterizing the geometry of the system being computed, whereas real contact pressure depends on the temperature, joint type (plastic or elastic), and surface mechanical properties of the materials [44]:

— for the elastic contact

$$P_{\rm r} = 2E \, \frac{R_{\rm a}}{S_{\rm m} t_{\rm m}} \,,$$

where S_m is the mean roughness asperity spacing of surface profile, m; t_m is the relative bearing length of the profile at the central line level (the ratio of the total length b_{mj} of sections cut off by the mean line drawn through the profile peaks to



Figure 7. Thermal contact resistance of an Al–Al plastic contact in a vacuum $[T_c = 550 \text{ K}, A_n = 10^{-2} \text{ m}, S_m = 10^{-5} \text{ m}, t_m = 0.8, 9c$ class of finish $(R_a = 0.2 \times 10^{-6} \text{ m}, R_z = 10^{-6} \text{ m})]$: (a) specific value calculated from formulas (5) - 1, (9) - 2, (11) - 3, (12) - 4, and (13) - 5; (b) total value (for constriction assigned to the real contact area A_r found as described in Ref. [44]) calculated from formulas (5) - 1, (9) - 2, (11) - 3, (12) - 4, and (13) - 5.



Figure 8. Thermal contact resistance of an Al–Al plastic contact in a vacuum $[T_c = 293 \text{ K}, A_n = 10^{-2} \text{ m}, S_m = 10^{-5} \text{ m}, t_m = 0.8, 14c \text{ class of finish}$ $(R_a = 0.006 \times 10^{-6} \text{ m}, R_z = 0.032 \times 10^{-6} \text{ m})]$: (a) specific value calculated from formulas (5)—1, (9)—2, (11)—3, (12)—4, and (13)—5; (b) total value (for constriction assigned to the real contact area A_r found as described in Ref. [44]) calculated from formulas (5)—1, (9)—2, (11)—3, (12)—4, and (13)—5.

the profile basal line length *l*):

$$t_{\rm m} = \frac{1}{l} \sum_{j=1}^n b_{{\rm m}j};$$

- for the plastic contact

 $P_{\rm r} = 0.8 H_T$.

If microhardness H_0 at room temperature is known, microhardness H_T at contact temperature T can be calculated using the following formula

$$H_T = H_0 \frac{1 - \Theta^{2/3}}{1 - \Theta_0^{2/3}},$$

where the dimensionless temperatures Θ , Θ_0 are determined with respect to melting temperature T_{melt} :

$$\Theta = \frac{T}{T_{\text{melt}}}, \quad \Theta_0 = \frac{T_0}{T_{\text{melt}}}.$$

The contact criterion (plastic or elastic) is defined by the quantity

$$\Pi = \frac{ER_{\rm a}}{H_T S_{\rm m}} \,.$$

The contact is termed plastic if $\Pi > 1/4$, and elastic if $\Pi \le 1/4$.

In the case of thermal interaction between different materials, contact pressure is calculated separately for each material. The real contact area is determined based on the minimal pressure principle, i.e., the lowest of the calculated values is taken as the real contact pressure, because deformation of a less thermostable material causes the contact spot area to increase. It may turn out that one of the materials retains elasticity at a given contact temperature, while the other becomes plastic. In such a case, the minimal pressure principle holds as well, i.e., the pressure exerted by the plastic material corresponding to the larger contact area is regarded as real contact pressure.

The above dependences may be used to evaluate thermal resistance in contacts of materials having smooth rough surfaces with a small average asperity height σ compared with the thickness of samples themselves. In such calculations, a heat flux tube model (Fig. 9a) is applied, for which the fictitious radius *r* is calculated from formula (6) for a single microcontact, and from formula (7) for total contact resistance. It is assumed that the constriction of heat flow lines is a one-step process and proceeds directly from tube radius *r* toward radius *a* of the real contact area A_r .

Such an assumption holds only if the surface has no loworder asperities. However, most applied studies deal with wavy rough surfaces where heat flow line constriction occurs in two steps: first from nominal area A_n of radius *r* to contour (apparent) wave-contact area A_a , and thereafter to the real area with radius *a* (see Fig. 2). In this case, the heat flux tube becomes more complicated and transforms into a two-step one (Fig. 9b). Thermal constriction resistances $R_{th, cn}$ is the sum of serial macroscale ($R_{th, lcn}$) and microscale ($R_{th, scn}$) constriction resistances:

$$R_{\rm th,\,cn} = R_{\rm th,\,lcn} + R_{\rm th,\,scn}$$
.

An advantage of the analytical models (5), (9), (11) is the possibility of using both macro- and microscale constrictions for computation purposes. It is enough to introduce intermediate fictitious radius r_a of the contour area and consider heat flow line constriction in the framework of the scheme $A_n(r) \rightarrow A_a(r_a) \rightarrow A_r(a)$. By way of example, Eqn (5) for a wavy rough surface is converted into

$$\begin{aligned} R_{\rm th,\,cn} &= \frac{r_{\rm a}}{2\lambda} \arctan\left(\frac{r}{r_{\rm a}} - 1\right) + \frac{a}{2\lambda} \arctan\left(\frac{r_{\rm a}}{a} - 1\right) \\ &= \frac{1}{2\lambda} \left[r_{\rm a} \arctan\left(\frac{r}{r_{\rm a}} - 1\right) + a \arctan\left(\frac{r_{\rm a}}{a} - 1\right) \right] \\ &= \frac{\delta_{\rm lcn} + \delta_{\rm scn}}{\lambda} = \frac{\delta_{\rm cn}}{\lambda} \,, \end{aligned}$$



Figure 9. Heat flux tube and schematic of thermal resistance: (a) smooth rough surfaces with equal nominal areas — one-step constriction; (b) wavy rough surfaces with different nominal areas — two-step constriction.

where δ_{lcn} , δ_{scn} are the thicknesses of flat walls thermally equivalent to perturbed zones formed by macro- and microconstrictions.

The third case is just as feasible: it corresponds to wavy unrough surfaces, the interaction between which is associated with macroconstriction alone. Although roughness is impossible to eliminate completely, an analytical expression for constriction resistances can be written in this case, too [it coincides with formula (5)] on the assumption of equality between the apparent and real areas: $A_a(r_a) = A_r(a), r_a = a$.

Moreover, combined cases are also conceivable in which smooth and wavy rough surfaces interact, with the one-step heat flux tube in one of them and the two-step tube in the other. Nominal cross section areas of interacting materials may differ, too. Analytical expressions allow constriction resistances to be computed independently for each solid body and can be easily adapted to any kind of interaction.

As a rule, empirical dependences for solids with equal nominal areas are constructed separately for macro- and microscale constrictions. To recall, formulas (12) and (13) permit calculating only microconstriction; hence, the necessity of additional expressions for wavy surfaces. For example, thermal macroconstriction resistance in a contact between two spherical surfaces of radii ρ_1 , ρ_2 ($\rho \ge \sigma$) is possible to find as [48, 49]

$$R_{\rm th,\,lcn,\,a} = \frac{1}{2\lambda_{\rm c}r_{\rm a}} \left(1 - \frac{r_{\rm a}}{r}\right)^{3/2}.$$
(14)

Specific thermal resistance $R_{\text{th, lcn}}$ is defined by the product of $R_{\text{th, lcn, a}}$ and apparent area A_a :

$$R_{\rm th, \, lcn} = R_{\rm th, \, lcn, \, a} A_{\rm a} = \frac{A_{\rm a}}{2\lambda_{\rm c} r_{\rm a}} \left(1 - \frac{r_{\rm a}}{r}\right)^{3/2}$$
$$= \frac{\pi r_{\rm a}^2}{2\lambda_{\rm c} r_{\rm a}} \left(1 - \frac{r_{\rm a}}{r}\right)^{3/2} = \frac{\pi r_{\rm a}}{2\lambda_{\rm c}} \left(1 - \frac{r_{\rm a}}{r}\right)^{3/2}.$$
 (15)

Radius r_a of the apparent area A_a is defined as

$$r_{\rm a} = \left(\frac{3N\rho}{4E'}\right)^{1/3},$$

where fictitious values of the radius of curvature ρ and elastic modulus E' are calculated in the following way:

$$\rho = \left(\frac{1}{\rho_1} + \frac{1}{\rho_2}\right)^{-1},$$

$$E' = \left(\frac{1 - v_1^2}{E_1} + \frac{1 - v_2^2}{E_2}\right)^{-1},$$

where E_1 , E_2 are elastic moduli of the contact pair, Pa, and v_1 , v_2 are the Poisson ratios. If the nominal surface areas of the samples are different, thermal constriction resistance in the contact of spherical surfaces takes the form [48, 49]

$$R_{\rm th, \, lcn, \, a} = \frac{1}{4\lambda_1 r_a} \left(1 - \frac{r_a}{r_1} \right)^{3/2} + \frac{1}{4\lambda_2 r_a} \left(1 - \frac{r_a}{r_2} \right)^{3/2}, \quad (16)$$

$$R_{\rm th, \, lcn} = \frac{\pi r_{\rm a}}{4\lambda_1} \left(1 - \frac{r_{\rm a}}{r_1} \right)^{3/2} + \frac{\pi r_{\rm a}}{4\lambda_2} \left(1 - \frac{r_{\rm a}}{r_2} \right)^{3/2}.$$
 (17)

Because relationships (14)–(17) are based on the heat flux tube model, they can be generalized and adapted to the calculation of both thermal resistances of a wider class of wavy surfaces and microscale constriction resistances by replacing r_a with *a*. Consideration of coefficient $\pi/2$ in formula (17) as the limiting value of arctangent in formula (5), and $(1 - a/r)^{3/2}$ as the constriction function Φ in formula (9), leads to expression (11) in the general form (as mentioned above, Φ can be different).

Thus, the main problem of thermal calculation of wavy rough surfaces consists in finding an apparent contact area A_a and the corresponding fictitious radius r_a (the method of A_a computation was described in Ref. [44]). Analytical expressions for constriction resistance have a number of advantages, such as their invariance with respect to macro- and microconstrictions, the possibility of separately calculating interacting solids and the related applicability to systems consisting of solids with different nominal areas. Empirical dependences can serve as criteria for the evaluation of analytical models obtained by generalization of the wealth of experimental data. Specifically, empirical dependences (12) were constructed based on more than 600 points corresponding to a wide spectrum of materials and classes of finish of surfaces [48, 49].

The above analytical expressions give values higher than the empirical ones. This may be due to the use of the maximum value of the shape factor $\psi = 1$ corresponding to round contact spots. Hence, the necessity of further studies of analytical models and their potential.

4. Heat flux rectification

In all the above formulas (4), (5), (9), (11)–(17), thermal contact resistance is expressed through the thermophysical properties of materials, their mechanical and geometric characteristics, or related parameters. A change in heat flux direction by permutation of temperature values at the outer borders of a system alters mean contact temperature and as a consequence thermal conduction resistances in both individual layers and perturbed zones of the material. In other words, the heat flux asymmetry effect occurs and thermal rectification takes place. Also apparent is the temperature dependence of thermomechanical properties: the real contact area changes upon heat flux inversion due to the difference between linear expansion coefficients of the materials; this change affects the relationship between heat flux values in the forward and backward directions. Important manifestations of this effect were observed independently by different authors in experimental studies [28, 48, 49, 55, 56].

A change of heat flux by interchanging boundary conditions of the first order in complex thermophysical systems composed of two or more objects in real contact with each other is observed in two characteristic cases [28]:

- a thermal joint consisting of different materials with similar or different surface properties, and

— a contact formed by identical materials with different surface properties.

Conclusions drawn from this observation suggest the cause of heat flux rectification. On the one hand, this effect is due to the difference between thermophysical properties of the interacting materials and their temperature dependences. Measurement of the asymmetry for contact pairs of MM59 brass–Armco iron and IX18H9T steel–alundum bonded by diffusion welding showed that the ratio of the forward-to-backward heat fluxes ($Q_{1,/}Q_{r}$) varies from 1.02 to 1.4 and is reproducible after rather a long time (several months). Selected results of this experimental study are presented in Table 2 [56].

Because the experiments involved practically ideally bonded samples (diffuse welding), the heat flux ratio roughly coincided with the density ratio; in other words, the influence of real contact area (consequently, mechanical and surface properties) on the effect of interest may be regarded in this case as insignificant. Considering that the thermal resistance of a multilayer wall with ideal contacts between the layers depends only on the difference in temperatures ΔT at the outer surfaces, thicknesses δ_m , and thermal conductivities λ_m of the layers [6]:

$$R_{
m th} = rac{\Delta T}{\sum_{m=1}^M \lambda_{
m m}/\delta_{
m m}} \; ,$$

where M is the number of layers (in this case 2), and layer thicknesses did not change over the course of the experiment, the above results confirm the dependence of thermal rectifica-

Table 2. Results of measurement of heat flux asymmetry effects.

Two-component specimen being studied	MM59 brass– Armco iron		IX18H9T steel– alundum		
Temperature at surface 1, °C	352.8	320.5	300.0	390.5	
Temperature at surface 2, °C	224.1	152.0	80.0	94.2	
Temperature difference at the outer surfaces of the samples, °C	128.7	168.5	220.0	296.3	
$\frac{\underline{Q}_{l}}{\underline{Q}_{r}} \approx \frac{q_{l}}{q_{r}}$	1.0533	1.0955	1.2088	1.2582	

tion on thermal conductivity:

$$K = \frac{\delta_1 \lambda_2}{\delta_2 \lambda_1} \, .$$

Coefficient *K* is a dimensionless variable used as the argument of dimensionless function f(K) (the ratio of the forward-tobackward heat fluxes, Q_1/Q_r):

$$f(K) = \frac{Q_1}{Q_r} \,. \tag{18}$$

Theoretical dependence f(K) for a certain two-component system at a constant temperature difference ΔT at the outer surfaces is shown in Fig. 10 [56]. There is an optimal K_0 value for a given contact pair that can be approached by varying thicknesses δ_1 and δ_2 of the materials. The variation will be accompanied by an alteration of average thermal conductivities of the layers as a sequel to a change in their mean temperatures, because mean contact temperature will be variable despite constant temperature at the outer surfaces.

The value of f_0 also varies depending on the relationship between thermal conductivities of the materials making up the contact pair. Possible variants of thermal conductivity behavior as a function of temperature are illustrated in Fig. 11. The maximum f_0 values at which heat flux rectification is especially pronounced correspond to the case exemplified in Fig. 11b, where thermal conductivities change oppositely. The rectification effect in Fig. 11a, b is less pronounced; in the case shown in Fig. 11d, the results may



Figure 10. Theoretical dependence f(K) for a contact pair at $\Delta T = \text{const.}$



Figure 11. Variants of varying thermal conductivities of contact pair materials as a function of temperature.

be different depending on preset temperature, meaning that the choice of a contact pair to ensure a maximum and stable heat flux rectification effect should be made using materials with highly variable thermal conductivity in response to temperature changes (as in Fig. 8b) and with the thicknesses corresponding to the optimal K value.

On the other hand, heat flux rectification in a contact of identical materials with different surface properties gives evidence of its dependence on surface and mechanical properties. It was shown in experiment that [28]:

— elastic strain does not lead to an appreciable change in the magnitude of the effect due to prolonged cyclic temperature inversion at the outer borders of a system, whereas plastic strain causes its reduction after a few cycles;

— heat flux rectification grows with a rise in contact pressure;

— it decreases in the presence of surface microasperities;

— heat flux rectification is greatly influenced by variations of surface properties and heat loading.

Experimental studies reveal some specific features but do not elucidate the physical basis of thermal rectification because of wide dispersion of the data observed, which is attributable to a variety of materials and surface characteristics of the samples. Hence, the importance of basic research for physical justification of experimental results.

Each of the above subgroups of theoretical studies offers its own explanation for heat flux rectification effect. The electron theory attributes heat flux rectification to the influence of the potential barrier formed in a contact between materials of different kinds on the electron heat flux, on the assumption that phonon conduction lacks the property of directionality. If $E_{w,1}$, $E_{w,2}$ are the work functions of metal surfaces and $E_{w,1} < E_{w,2}$, the electron flow is directed from metal 1 to metal 2 because electrons at the conduction boundary of metal 1 are closer to the potential barrier. If $E_{w,1} > E_{w,2}$, the electron flow is directed from metal 2 to metal 1. Because the work functions depend on the surface geometry, as well as on the properties of surface films and sample materials, thermal rectification is a function of these parameters, too [38, 51, 57]. Although this assertion is valid, the electron theory does not explain heat flux rectification in a

uniform contact where charge carriers in the interacting metals reside at the same energy level. Moreover, this theory fails to account for the rectification effect in nonmetallic contacts where only phonon thermal conductivity is present. Hence it follows that the hypothesis for the dependence of thermal rectification on the potential barrier associated with the difference between work functions of the interacting metals is applicable only to electron thermal conductivity in contacts of metals and semiconductors.

The same conclusions apply to 'film' theories attributing the heat flux rectification effect to the influence of surface films [13]. Dielectric and semiconducting films actually form a significant potential barrier for carriers of electric current and have high electrical resistance [16]. However, the thermal resistance of such films is as a rule low due to their small thickness, and its changes upon inversion of the heat flow are insignificant compared with overall contact resistance and its phonon constituents (running to a few percent of the mean film resistance). Because a change in the heat flux in the case of boundary temperature inversion may be as large as 40% [27], it is the phonon constituent of thermal contact resistance that is responsible for thermal rectification, even though films may just as well influence electron thermal conductivity.

'Microscopic' and 'macroscopic' theories that postulate the dependence of contact conduction on the surface and mechanical properties of materials explain the rectification effect by variation of contact micro- and macroareas, leading to changes in micro- and macroconstriction resistances. There are several types of contacts, depending on the surface structure of the materials. They can be either wavy with a mean asperity height a few orders of magnitude smaller than the mean waviness height or rough with the waviness height commensurate with that of asperities (i.e., the interacting surfaces are almost ideally flat). The higher thermal resistance is believed to correspond to a heat flow direction away from the material with lower thermal conductivity in the former case, and toward such a material in the latter [51, 58].

The theory of micro- and macroconstrictions was extended to the methods of calculation of contact heat exchange, taking into account the effects of thermal stress in the interface on the real contact area. The thermal stress is proportional to the product of linear expansion coefficient β and difference ΔT between maximum and minimum temperatures at the sample's contact surface [51, 59]:

$$\varepsilon \sim \beta \Delta T$$
.

Because ΔT is inversely proportional to the thermal conductivity λ of the material, one finds

$$\varepsilon \sim \frac{\beta}{\lambda}$$
.

It was shown in experiment that thermal conductance in the contacts between different types of materials increases when the heat flow is directed from the material with higher thermal stress to the one with lower stress [51]. The distance Δ between mean planes of contacting surfaces, namely

$$\Delta = (-1)^{i+1} \frac{r^2 \bar{q}}{2} \left(\frac{\alpha_1}{\lambda_1} - \frac{\alpha_2}{\lambda_3} \right),$$

was proposed as a theoretical criterion for maximum heat flux direction [51, 60] (\bar{q} is the mean heat flow density through a contact taking account of the flow sign, W m⁻²; *r* is the sample



Figure 12. Schematics of profiles of the contacting ends of cylindrical samples with a heat flux across them.

radius, m, and *i* is the sample's identification number). When the absolute value of Δ is larger than asperities at the interacting surfaces, contact thermal conductance is higher for the heat flow directed away from the material with lower thermal stress. If Δ is smaller than the average surface asperity size, maximum contact conductance occurs when heat is transferred from the material with higher thermal stress [60].

The exact solution to the thermoelasticity problem for a cylinder was proposed to quantitatively describe the effect of heat flux magnitude and direction on thermal contact resistance. It led to the conclusion that the surface profile at the base end of the cylinder depends neither on heat transfer at its cap end nor on the temperature profile of the end being cooled; indeed, it was totally determined by heat flux magnitude and direction [18]. If heat enters an end, the flow is positive and the end becomes convex; if heat is emitted from an end of a cylinder, it becomes concave. When samples of identical materials are in contact, the radii of convexity and concavity of the interacting ends coincide, and thermal resistance is due only to heat flux constriction toward contact microspots (Fig. 12). Because the mean size of microspots shows but weak dependence on contact pressure, the quality of surface processing, and the type of materials, thermal contact resistance is practically independent of the heat flow direction for thermal interaction between identical materials. When samples of different materials are in contact, the contact surface depends on the ratio of radii of curvature of the contiguous ends. The microwaviness of end surfaces created by thermal expansion of the materials may form a contact either within a single macrospot or within a macroring. The above patterns hold upon fulfilling the condition [18]

$$\frac{\bar{q}}{P_{\rm n}} \geqslant \frac{3\pi}{2} \, \frac{\lambda_2}{\beta_2 E r} \, ,$$

where \bar{q} is the mean heat flow density across the contact, W m⁻²; P_n is compressive pressure, Pa; λ_2 is the thermal conductivity of the heat-absorbing material, W (m K)⁻¹; β_2 is the coefficient of thermal expansion of the heat-absorbing material, K⁻¹; *E* is the reduced elastic modulus, Pa, and *r* is the cylinder radius, m. When this condition is not fulfilled, the microspot size is commensurable with the end sizes and thermal conductance of the contact (in a vacuum) is totally determined by the resistance of constriction to contact microspots.

5. Thermal contact under a nonstationary regime

Microconstriction of heat flow lines to the real contact zone occurs in the immediate vicinity of a contact median plane, at a distance of order [33]

$$\delta_{\rm cn} \sim \left(\frac{A_{\rm n}}{n_{\rm r}}\right)^{1/2}$$

where A_n is the nominal contact area, m^2 , and n_r is the number of real contact spots. The layer of material bounded by the contact median plane on the one side, and the plane spaced δ_{cn} apart on the other side, is referred to as the perturbation zone. More appropriate δ_{cn} values can be found from formulas (5) or (9), depending on whether the perturbation zone thickness remains constant or varies. Microconstriction in this zone enters a steady-state regime during a certain characteristic time interval called relaxation time:

$$\tau_1 = \frac{\Delta^2}{a_1} = \frac{A_a}{n_r a_1} \text{ for body } 1, \ \tau_2 = \frac{\Delta^2}{a_2} = \frac{A_a}{n_r a_2} \text{ for body } 2,$$
(19)

where a_1 , a_2 are the thermal diffusivities of materials 1 and 2, m² s⁻¹. For transient thermal regimes with characteristic time τ_c in excess of relaxation time τ , relation (3) holds true; this means that such nonstationary processes are at each moment described by the classical theory of thermal conduction. When the characteristic time of the nonstationary regime is smaller than the microconstriction time, simulation of such processes requires an additional analysis based on a theory taking account of interactions between microparticles [44].

Nevertheless, attempts were undertaken to construct phenomenological models of a nonstationary real contact, making it possible to evaluate the effect of the perturbation zone on the temperature field and heat flow under the relaxation regime by introducing a fictitious thermal conductivity and thermal capacity of the perturbation zone. The nonuniform layer of a real contact was replaced by an equally thick uniform wall with ideal solid-solid contacts, having the internal energy of the nonuniform layer [61, 62]. The nonuniformity of the real contact was taken into account by dividing the fictitious layer into zones with different thermal conductivities (Fig. 13): zone 3 simulates thermal conductivity across real contact spots, and zone 4 specifies properties of the medium in intercontact gaps. Thermal conductance of the equivalent wall is the sum of parallel conductances $\alpha_{\text{th},3,a}$ and $\alpha_{th, 4, a}$:

$$\begin{split} \alpha_{\mathrm{th,\,c,\,a}} &= \alpha_{\mathrm{th,\,3,\,a}} + \alpha_{\mathrm{th,\,4,\,a}} \Leftrightarrow \frac{1}{R_{\mathrm{th,\,c,\,a}}} = \frac{1}{R_{\mathrm{th,\,3,\,a}}} + \frac{1}{R_{\mathrm{th,\,4,\,a}}} \\ &\Leftrightarrow R_{\mathrm{th,\,c}} = \left(\frac{1}{R_{\mathrm{th,\,3,\,a}}} + \frac{1}{R_{\mathrm{th,\,4,\,a}}}\right)^{-1}. \end{split}$$

The problem may be confined to a one-dimensional case by advancing hypotheses considering boundary conditions and temperature field [62]:

— at any point on the side surface of zone D, the heat flux is zero, namely

$$\frac{\partial T}{\partial \mathbf{n}} = 0;$$

— all media being considered are in ideal contact $(R_{\text{th},i} \rightarrow 0)$;



Figure 13. Diagram showing the replacement of the perturbation zone in a real contact by a thermally equivalent heterogeneous layer.

— temperature distribution is uniform over the surfaces $P_1, P_2;$

 — thermal conductance in zone D is assumed to be linear. Final expressions for thermal capacity and bulk thermal conductivity of the equivalent layer are written out in the form [62]

$$\lambda' = \frac{\lambda_3 A_3 \,\partial \bar{T}_3(x,\tau)/\partial x + \lambda_4 A_4 \,\partial \bar{T}_4(x,\tau)/\partial x}{A_3 \,\partial \bar{T}_3(x,\tau)/\partial x + A_4 \,\partial \bar{T}_4(x,\tau)/\partial x} \,, \tag{20}$$

$$c'\rho' = \frac{c_3\rho_3 A_3 \,\partial \bar{T}_3(x,\tau)/\partial \tau + c_4\rho_4 A_4 \,\partial \bar{T}_4(x,\tau)/\partial \tau}{A_3 \,\partial \bar{T}_3(x,\tau)/\partial \tau + A_4 \,\partial \bar{T}_4(x,\tau)/\partial \tau} \,. \tag{21}$$

Thus, calculation of λ' and $c'\rho'$ requires knowledge of temperatures $\overline{T}_3(x,\tau)$, $\overline{T}_4(x,\tau)$ derived from these parameters; in other words, the problem is formulated incorrectly from the standpoint of mathematical physics [63]. Nevertheless, it is possible to roughly determine the thermophysical properties of the equivalent wall.

This purpose can be achieved by introducing a local separation $\alpha(x, t)$ of the heat flux that is the ratio of the heat flux $Q_3(x, t)$ across the area A_3 to the total flux Q(x, t) across the section Σ :

$$\alpha(x,t) = \frac{Q_3(x,\tau)}{Q(x,\tau)} \,.$$

Then, the heat flux $Q_4(x, t)$ across the section A_4 can be found as

$$Q_4(x,\tau) = Q(x,\tau) - Q_3(x,\tau) = \left[1 - \alpha(x,t)\right] Q(x,\tau)$$

and thermal conductivity λ' , according to formula (20), as

$$\begin{aligned} \mathcal{U}'(x,t) &= \frac{Q_3(x,\tau) + Q_4(x,\tau)}{Q_3(x,\tau)/\lambda_3 + Q_4(x,\tau)/\lambda_4} \\ &= \frac{1}{\alpha(x,\tau)/\lambda_3 + (1-\alpha(x,\tau))/\lambda_4} \,. \end{aligned}$$

This means that when there is a small variation in $\alpha(x, \tau)$, the approximate value of fictitious thermal conductivity may be defined in the following way:

$$\lambda'(x,t) \approx \lambda_{\rm a}$$
,

where λ_a is the mean fictitious heat conductivity, W (m K)⁻¹, of a nonuniform layer, measured under a stationary regime.

The approximate calculation of fictitious bulk thermal capacity is based on the assumption of rather close rates of variation of average temperatures $\overline{T}_3(x,\tau)$, $\overline{T}_4(x,\tau)$:

$$\frac{\partial \bar{T}_3(x,\tau)}{\partial \tau} \approx \frac{\partial \bar{T}_4(x,\tau)}{\partial \tau} \,,$$

i.e., according to expression (21), one obtains

$$c'\rho' \approx \frac{c_3\rho_3A_3 + c_4\rho_4A_4}{A_3 + A_4} = c_a\rho_a \,,$$

where $c_a \rho_a$ is the fictitious bulk thermal capacity, J (m³ K)⁻¹, of a nonuniform layer in the stationary regime. This heterogeneous layer model is a linear one because $c_a \rho_a$ and λ_a are constant quantities.

In the relaxation regime starting from the point in time $\tau = 0$, the temperature at each point *M* of the system with coordinate x_M may be represented as

$$T(x_M,\tau) = \sum_{j=1}^{\infty} Q_j(x_M) \exp\left(-m_j\tau\right) + F(x_M),$$

where $F(x_M)$ is the temperature distribution under the stationary regime, K, and m_j are the coefficients of a series independent at each point M, s⁻¹.Till the point in time of order $1/m_1 = 1/m$, a change in temperature is correctly described by the first term of this series:

$$\bar{T}_k(x,\tau) = \bar{Q}_k(x) \exp\left(-m\tau\right) + \bar{F}_k(x), \ k = 1, 2, 3, 4.$$
 (22)

The thermal conductivity and bulk thermal capacity of the equivalent layer in the relaxation regime are determined by substituting temperature field (22) into expressions (20), (21). In the specific case of $\bar{F}_k = \text{const}$, these thermophysical properties are time- and temperature-independent continuous functions of the spatial coordinate:

$$\lambda'(x,\tau) = \frac{\lambda_3 A_3 \,\mathrm{d}Q_3(x)/\,\mathrm{d}x + \lambda_4 A_4 \,\mathrm{d}Q_4(x)/\,\mathrm{d}x}{A_3 \,\mathrm{d}\bar{Q}_3(x)/\,\mathrm{d}x + A_4 \,\mathrm{d}\bar{Q}_4(x)/\,\mathrm{d}x} = \lambda'(x)\,,$$
(23)

$$c'\rho'(x,\tau) = \frac{c_3\rho_3A_3Q_3(x) + c_4\rho_4A_4Q_4(x)}{A_3\bar{Q}_3(x) + A_4\bar{Q}_4(x)} = c'\rho'(x).$$
(24)

In the general case of $\bar{F}_k \neq \text{const}$, expression (24) for bulk thermal capacity is retained, but the simplification inserted by Eqn (23) is no longer suitable for the description of fictitious thermal conductivity that, under the relaxation regime, must tend to its asymptotic limit in the stationary regime [62]:

$$\lambda'(x,\tau) = \frac{\lambda_3 A_3 \, \mathrm{d}F_3(x)/\mathrm{d}x + \lambda_4 A_4 \, \mathrm{d}F_4(x)/\mathrm{d}x}{A_3 \, \mathrm{d}\bar{F}_3(x)/\mathrm{d}x + A_4 \, \mathrm{d}\bar{F}_4(x)/\mathrm{d}x} \to \lambda'_\infty(x) \,.$$

Thus, the equivalent wall model is applicable only to the description of nonstationary processes in the perturbation

zone near the stationary state when fictitious thermal conductivity is close to its value in the steady-state regime. This method and the equivalent wall model cannot be used to calculate fictitious thermal conductivity in nonstationary processes with a characteristic time smaller than the microconstriction time.

Of interest in this context is an approach based on the methods of irreversible thermodynamics applied to the description of media with internal parameters of state and rate type media, the approach into which the heat propagation rate is introduced [64]. A similar parameter is utilized in the theory of thermal conduction of discrete media, treating thermal conduction as a process of heat wave propagation with given energies and momenta [53, 65, 66].

6. Thermal conduction in nanosystems

The development of nanotechnologies and the wide application of nanomaterials excite keen interest in the mechanisms of heat transfer in nano-sized structures. Such structures underlie current state-of-the-art technological advances in the fields of silicon-based electronics, the manufacture of carbon nanotubes, semiconducting quantum lattices, polymer nanocomposites, multilayer films and coatings, etc. Some devices (computer processors, semiconductor lasers) need maximum thermal conductance, while others (thermal diodes, thermoelectrical materials) need only the minimum. Experiments have demonstrated that the proximity of contact surfaces and an extremely small volume of interfaces substantially alter heat transfer, thereby complicating thermal regulation [67]. These issues require different approaches, depending on the dielectric properties of the materials used in particular devices and determining thermal conduction mechanisms, viz. electronic (in metals), phononic (in nonmetals), or mixed (in metals, semiconductors). The greatest difficulties are posed by interfaces where thermal interactions between solids with different dielectric properties (e.g., between metals and dielectrics or semiconductors) occur. These cases require special consideration of spatially separated electron and phonon conductances, followed by examination of interactions between their carriers in a contact. In materials with mixed thermal conduction, electrons and phonons are coincident in space, which necessitates consideration of electron-phonon interaction within the confines of a same medium.

Phonons as the major heat flux carriers in nonmetals are 'quasiparticles' of elastic waves propagating by virtue of lattice oscillations. They fall within a wide frequency and mean free path (prior to scattering) ranges. The mean free path of 1–100 nm at room temperature is commensurate with the structure size of the material and sometimes with the heat wavelength. None of the existing analytical theories fully describes the wave nature of phonons. This fact underlies the striking discrepancy between theoretical and experimental findings. Moreover, a number of fundamental problems, such as determination of temperature along phonon mean free paths, remain unresolved.

There are two main approaches to theoretical investigations into phonon thermal conductivity, besides Fourier's law [67]:

numerical solution of the Boltzmann equation;

— simulation of thermal conduction at the atomic level.

The majority of atomic thermal conduction models have been constructed by molecular dynamics methods based on Newton's equations of motion and, as a rule, empirical expressions for the interatomic interaction potential. It is a classical approach that can be employed to study thermal processes in solids at temperatures above the Debye temperature. It also disregards electron-phonon interactions in metals and semiconductors, but is fairly suitable for simulating phonon thermal conductivity. The following molecular dynamics methods are most frequently used for the purpose [67]:

— Green–Kubo method for studying lattice thermal vibrations in the presence of a heat flow;

— the 'direct method' reproducing the process of application of the temperature gradient (of the order of 10^9 K m⁻¹) to a system and evaluating thermal conductivity from the Fourier law.

Both methods allow thermal conductivity to be calculated with a roughly similar accuracy (around 20%), but the latter has an additional advantage making it possible to compute thermal contact resistance for multilayer systems.

Numerical models of heat exchange in a solid–solid contact demonstrate the presence of intrinsic thermal resistance even in mechanically ideal interfaces (absence of constriction) of crystals with a diamondlike structure and differing only in atomic masses. The corresponding thermal conductance for different boundary conditions is $0.8-0.9 \text{ GW m}^{-2} \text{ K}^{-1}$; for analogous Si crystals, it ranges $0.85-1.53 \text{ GW m}^{-2} \text{ K}^{-1}$ (Fig. 14). The equivalent thickness of a perfect crystal with the same thermal resistance is on the order of 100 nm [67].

A sharp rise in the temperature gradient occurs in the interface region due to phonon scattering as they cross the crystal-crystal interface. Phonons reflected from the potential barrier have an energy different from that of the passing phonons, with the difference increasing as the interface is approached. This leads to a rise in the mean phonon energy gradient and, as a consequence, accounts for the greater temperature gradient near the interface. The temperature of reflected phonons is termed boundary temperature. The difference between boundary temperature and the results of linear extrapolation of temperature distribution inside the medium is directly proportional to the ratio of heat flux to phonon mean free path and thermal conductivity of the material. In other words, this quantity determines the temperature gradient and thermal conductance $\alpha_{th,c}$ of atomic layers adjacent to the interface.



Figure 14. Temperature profile calculated for a two-layer Si crystal (the 25-nm-thick sample contains 840 atoms along the computed axis); computation time is 1 ns.

The exact expression for calculating $\alpha_{th,c}$ was proposed by D Young and H Maris (see Ref. [67]):

$$\alpha_{\rm th,c}(T) = \int C(\omega,T) \langle v(\omega) \rangle \langle t(\omega) \rangle \, \mathrm{d}\omega \,,$$

where ω is the heat wave frequency, Hz; $C(\omega, T)$ is a specific function characterizing the state of phonons and being determined from the Bose–Einstein distribution, J s m⁻³ K⁻¹; $\langle v(\omega) \rangle$ is the phase velocity component normal to the interface, m s⁻¹; $\langle t(\omega) \rangle$ is the transition coefficient, and $\langle v(\omega) \rangle$ and $\langle t(\omega) \rangle$ are averaged over the entire frequency range and all wave vectors directed either perpendicular or at an angle to the interface. Young and Maris showed that $\langle t(\omega) \rangle$ monotonically decreases with increasing ω . This result differs from the classical observation that the transition coefficient weakly depends on wave frequency up to its limiting value equal to the maximum frequency of a softer material.

The classical models permitting us to determine the transition coefficient include:

— the acoustic model, in accordance with which thermal resistance of an ideal contact is a consequence of different densities ρ and velocities of sound *a* of interacting materials α and β [67]:

$$\langle t_{\alpha\beta} \rangle = \frac{4Z_{\alpha}Z_{\beta}}{\left(Z_{\alpha} + Z_{\beta}\right)^2} ,$$

where $Z = \rho a$ is the acoustic impedance, kg (m s)⁻¹;

— the diffusion model postulating that all phonons colliding in the interface 'forget' their movements prior to scattering event, the probability of which is proportional to the density of phonon states

Both molecular dynamics and quantum mechanics make use of the thermodynamic definition of temperature, i.e., they consider this parameter as making sense for macroscopic systems distinctive for the statistical reproducibility of their related events and measurements. Moreover, a new notion is introduced in quantum mechanics: it is the notion of a particle ensemble in which particles exist *independently* from one another under similar macroscopic conditions. The result of measurement of the state of a quantum ensemble coincides with the result of many successive measurements of the states of its elements, i.e., the key factor is not the number of elements but the number of experiments that can be made either using a large number of particles for a short time interval or a small number of them during a long period [68].

The temperature is defined as a quantity related to the mean kinetic energy of the system obtained in N measurements [67]:

$$\langle \varepsilon_i \rangle = \frac{\mu}{2N} \sum_{i=1}^N v_i^2 = \left\langle \frac{1}{2} \mu v_i^2 \right\rangle, \tag{25}$$

where μ is the atomic mass, kg. The character of the interplay depends on the computation method involved:

— the molecular dynamics method based on Newton's mechanics uses the classical relation [67]

$$\left\langle \frac{1}{2} \mu v_i^2 \right\rangle = \left\langle \varepsilon_i \right\rangle = \frac{3}{2} k T_i;$$

— quantum mechanics assumes the average excitation energy of an atomic system to be equal to the energy of a phonon with wave vector \mathbf{q} and polarization γ for Bose–Einstein statistics [67]:

$$\left\langle \frac{1}{2} \mu v_i^2 \right\rangle = \frac{1}{4N} \sum_{\gamma, \mathbf{q}} \hbar \omega_{\gamma}(\mathbf{q}) \,\xi^{(i)\,2}(\gamma, \mathbf{q}) \\ \times \left\{ \frac{2}{\exp\left[\hbar \omega_{\lambda}(\mathbf{q})/(kT_i)\right] - 1} + 1 \right\},$$
(26)

where $\xi^{(i)2}$ are the squares of polarization vector components normalized in such a way that

$$\sum_{\gamma} \xi^{(i)\,2}(\gamma,\mathbf{q}) = 3\,.$$

For high temperatures (above 1000 K), at which $kT \ge \hbar \omega_{\gamma}(\mathbf{q})$, the state of Bose particles is approximated by the following equation [67]:

$$\frac{2}{\exp\left[\hbar\omega_{\lambda}(\mathbf{q})/(kT_{i})\right]-1}+1\approx 2\,\frac{kT_{i}}{\hbar\omega_{\lambda}(\mathbf{q})}$$

In this case, expression (26) is converted to Eqn (25) and quantum mechanics predicts the same result as molecular dynamics. Temperatures falling in the range of 300 to 1000 K and being calculated from formulas (25) and (26), are significantly different. Expression (26) is preferred in this range since the quantum-mechanical method is more applicable to the low-temperature region.

The temperature of a classical system is known at each point of its trajectory, whereas the quantum approach establishes a minimal size of the system (phonon mean free path) for which it is possible to compute the temperature. Phonon distribution differs in systems with different temperatures and can vary as a result of phonon scattering during the interaction between the systems: a single phonon usually splits into two or two phonons fuse together. Low- and highfrequency phonons have large and small mean free paths, respectively. The phonon mean free path is referred to as Casimir's boundary. As a rule, it is bigger than the size of cells simulated by molecular dynamics methods.

The sizes of nanoscale systems being commensurable with the phonon mean free path, the question arises as to the possibility of determining local temperature in quantum mechanics. Equation (26) relating temperature to phonon excitation energy and frequency does not allow temperature discontinuity between different atomic layers, in conflict with the picture in Fig. 14. These results can be obtained in an experiment on X-ray scattering from the corresponding atomic lattices. Given the thickness of the atomic layer is smaller than the phonon mean free path, it is impossible to determine the temperature within the confines of the layer using the above quantum definition. The Landauer formalism assuming heat transfer from one reservoir to another is equally inefficient, the mean free path being much smaller than the distance between the reservoirs [67].

Another quantum approach to temperature determination relates temperature to mean frequency of atomic oscillations [65, 69] by introducing the notion of a 'quasiparticle' whose kinetic and total energies are equal to the respective mean energies of a given atomic system. The quasiparticle is regarded in coordinate and momentum frames of reference, the origins of which coincide with the centers of probability distributions of the given quantities $(\bar{x} = 0, \bar{p} = 0)$. In such a choice of the frames of reference, the mean squares of coordinates and momenta equal their root-mean-square deviations $(\Delta x)^2$ and $(\Delta p)^2$ [66]:

$$\overline{(\Delta x)^2} = \overline{(x - \bar{x})^2} = \overline{x^2}, \quad \overline{(\Delta p)^2} = \overline{(p - \bar{p})^2} = \overline{p^2}.$$

Then, the average kinetic energy $\bar{\epsilon}$ proves to be equal to the kinetic energy uncertainty (square root of standard deviation) [65]:

$$\bar{\varepsilon} = \frac{\overline{(p)^2}}{2\mu} = \frac{\overline{(\Delta p)^2}}{2\mu} = \sqrt{\overline{(\Delta \varepsilon)^2}} = |\overline{\Delta \varepsilon}|, \text{ i.e., } |\overline{\Delta \varepsilon}| = \frac{1}{2} kT,$$
(27)

where μ is the particle mass, and *T* is the thermodynamic temperature independent of the number of degrees of freedom of the system. According to formula (27), the absolute temperature cannot be equal to zero because the infinitesimal uncertainty of the momentum corresponds to the infinite uncertainty of the coordinate, having no physical sense (the Heisenberg uncertainty relation):

$$\overline{(\Delta p)^{2}(\Delta x)^{2}} \ge \frac{\hbar^{2}}{4} \Leftrightarrow 2\mu |\overline{\Delta \varepsilon}| \overline{(\Delta x)^{2}} \ge \frac{\hbar^{2}}{4}$$
$$\Leftrightarrow \mu k T \overline{(\Delta x)^{2}} \ge \frac{\hbar^{2}}{4} \Leftrightarrow T \overline{(\Delta x)^{2}} \ge \frac{\hbar^{2}}{4\mu k} \Leftrightarrow T \ge \frac{\hbar^{2}}{4\mu k} \frac{1}{(\Delta x)^{2}},$$

in agreement with the third law of thermodynamics.

This approach yields the expression for absolute temperature in the form [65, 66, 69]

$$T = f(E_0) = f(\hbar\omega_0), \qquad (28)$$

where E_0 is the total energy, J, of a quasiparticle characterizing the state of a homogeneous system composed of '0' particles, and ω_0 is the cyclic frequency of thermal oscillations of the quasiparticle, Hz.

Temperatures of atomic a and b layers in an ideal contact are identical and equal to a certain T_{ab} value only under thermodynamic equilibrium conditions. Bearing in mind the relationship (28) between the particle energy and temperature, one may argue that particles a and b in these conditions should occupy the energy level E_{ab} . In all other cases, E_{ab} represents a limit to which total energies of the particles in atomic layers of an ideal contact approach (Fig. 15). Particles of the system a from which the heat flux is transferred occupy



Figure 15. Periodic energy transitions of particles in atomic layers of homogeneous systems a and b that are in ideal contact.

a higher energy level than E_{ab} :

$$E_{\rm a} = E_{\rm ab} + \Delta E_{\rm a} \,,$$

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and particles of the system b occupy a lower level:

$$E_{\rm b} = E_{\rm ab} - \Delta E_{\rm b} \,.$$

Energy transfer from the system a to system b corresponds to transition I of particles a and b to the level E_{ab} .

On the other hand, particles a and b interact with particles of their respective systems. Therefore, they do not stay at level E_{ab} (transition 2): a-particle moves to a more excited state, and b-particle to a less exited state (E_a and E_b , respectively). This double 1-2 transition results in a spatial spread of thermal energy. The time of double transition equals the doubled time $\Delta \tau$ of one-way transition. Identical particles a and b (belonging to one and the same individual substance) have equal excitation energies:

$$\Delta E_{\rm a} = \Delta E_{\rm b}$$
.

Because periodic energy transitions of the particles around an equilibrium state result in the spatial spread of energy and occur without matter transfer, thermal conductivity at the atomic level is essentially the propagation of heat waves [53].

The above-considered picture describes the thermal conduction mechanism in matter at the quantum level and extends A F Ioffe's hypothesis according to which, when the phonon mean free path is equal to or smaller than the lattice constant, heat spreads only by energy exchange between neighboring atoms [70].

If the phonon mean free path is much greater than the lattice size, the main factor influencing thermal conductivity is phonon scattering. A F Ioffe suggested that the main sources of phonon scattering in this case might be anharmonicity density fluctuations of thermal vibrations. He proposed the following formula (see Ref. [70]):

$$\lambda_{\rm ph} = \frac{v_{\rm ph}}{3} \left[g_0 \left(T - \frac{\theta}{3} \right) \right]^{-1},$$

where λ_{ph} is the phonon thermal conductivity, W (m K)⁻¹; g_0 is the anharmonicity coefficient, m² J⁻¹; v_{ph} is the mean velocity of phonons, m s⁻¹, and θ is the Debye temperature, K. The Debye temperature reflects the state of a solid in which all lattice vibration modes (degrees of freedom) are excited. A further rise in temperature produces no new modes but enhances mean vibration energy due to greater vibration amplitudes of the existing modes. The Debye temperature is given by

$$\theta = \frac{\hbar\omega_{\max}}{k}$$

where ω_{max} is the maximum cyclic atomic vibration frequency in a solid, Hz. The value of g_0 is found in experiment but can be just as well derived from calculations based on the fact that the Grünaisen constant computed analytically depends on anharmonism of vibrations and is in fact a modified anharmonicity coefficient [70].

Metals and crystalline semiconductors exhibit not only phonon but also electron thermal conductivity; the latter prevails in metals. The kinetic theory of electron thermal conductivity is based on the hypothesis for the existence of an electron gas whose particles are electrons. Following the Debye kinetic formula, the thermal conductivity of a gas is given by [70]

$$\lambda = \frac{1}{3} c_v v l \,,$$

where c_v is the bulk thermal capacity, J m⁻³ K⁻¹; v is the mean velocity of particles, m s⁻¹, and *l* is the mean free path, m. In the absence of electric current, the Debye formula can be converted, using the Boltzmann equation and neglecting certain factors, into an expression called the Wiedemann–Franz law [70]:

$$\lambda_{\rm e} = \frac{\pi^2}{3} \left(\frac{k}{e}\right)^2 \sigma T, \tag{29}$$

where σ is the specific electrical conductance, Ω^{-1} m⁻¹. This expression represented in the general form is known as the Wiedemann–Franz–Lorentz law [70]:

$$\lambda_{\rm e} = L\sigma T \,, \tag{30}$$

where *L* is the Lorentz number, $J^2 C^{-2} K^{-2}$. The universal character of expression (30) is due to the possibility of describing unaccounted peculiarities of electron behavior using different *L* values. Experimental studies have confirmed the validity of the Wiedemann–Franz–Lorentz law in the form (30) for all metals, and in the form (29) for many of them. Certain metals undergo deviation from relationship (29) over the entire temperature range, whereas others do so only at selected temperatures. The Lorentz number of semiconducting materials strongly depends on the interband scattering, which also accounts for the necessity of invoking special computation techniques.

The main mechanisms of thermal conduction, such as electronic and phononic ones, are supplemented by auxiliary mechanisms (bipolar diffusion, electromagnetic radiation, heat transfer by highly excited carriers and spin waves); collectively, they account for the total thermal conduction of a given material. Electron–phonon interaction manifests itself in metal–semiconductor contacts, too.

Generally speaking, experiments confirm the applicability of the additivity rule to overall thermal conductivity of solids [70]:

$$\lambda = \sum_i \lambda_i \,,$$

where λ_i is the constituent of total thermal conductivity, W (m K)⁻¹.

Thus, studies of thermal conductance in nanosystems are part of an actively developing field of research concerning the theory of thermal conduction in solids. A number of its aspects await clarification, e.g., validity limits of thermodynamic temperature, mechanisms of thermal conduction in structures smaller than the phonon mean free path, contact thermal conductivity of nanosystems, thermal resistance of ideal contacts, heat transfer across surface nanofilms, and some others. Solving these problems by the methods of thermal physics and solid-state physics is a logical continuation of these theories. At the same time, many solutions obtained for solids prove inaccurate when applied to nanoscale interpretation of thermal conduction processes (for example, the Wiedemann–Franz–Lorentz law) and require additional analysis with the use of up-to-date quantum-mechanical methods. Many experimental findings, such as the existence of thermal resistance in ideal contacts, need theoretical interpretation and can be introduced into the manufacturing of nanomaterials and thermal regulation of nanosystems.

7. Heat transfer in nanofilms

Semiconducting and dielectric films that naturally form on metallic surfaces in the air usually have a negative effect on the thermal conductivity of multilayer systems that needs to be taken into account [50]. However, it is possible to manufacture surface nanofilms for specialized purposes, first and foremost for use in microelectronics (silicon insulators, multilayer electronic devices, semiconducting or dielectric membranes) [67]. In all these cases, the thermal conductance of the films should be clearly specified and, if possible, amenable to regulation.

Films formed in natural conditions by gas adsorption fall into an adhesive type. It remains uncertain whether such films exist for long or undergo rapid transformation into oxide films. The thickness of the adhesive layer (roughly 0.7 nm) is somewhat larger than that of the monomolecular layer, and the film covers the entire surface of the metal. So-called tarnish films usually consist of oxide or sulfide films on the metal surface and have a thickness of a few nanometers. They grow slowly at room temperature. As the temperature rises, both film thickness and growth rate increase. For T > 573 K and T > 1073 K, the growth rate obeys parabolic and linear laws, respectively. The growth practically stops after the film becomes 6–10 nm thick (at room temperature); this is sufficient to protect the material from further oxidation. The thickness of oxide films over noble metals is very small. Gold is usually coated with a single adhesive layer of oxygen. As shown in experiment, surface films on steel, aluminium, copper, silver, and gold are readily destroyed [50].

The thickness of artificial films utilized in microelectronics comprises several dozen or hundred nanometers. The main factors affecting their thermal conductivity are thickness, homogeneity and structure of the material, presence of admixtures, and temperature. Single crystals over 500 nm in thickness (well above the Casimir boundary) exhibit the highest thermal conductivity. A decrease in thickness of the single crystal impairs its thermal conductivity. Impurities cause distortion of the crystal structure, also accompanied by impairment of thermal conductivity.

The thermal conductivity of polycrystalline films of the same thickness is much lower but admixtures increase it. The most widely used are silicon (Si) and silicon dioxide (SiO₂) films. Also in use are GaAs, Ge, and AlAs films [70].

It is generally believed that the small thickness of the films is responsible for their negligibly low thermal conduction resistance equaling the film thickness (δ_f)-to-thermal conductivity (λ_f) ratio:

$$R_{\rm th,\,f} = \frac{\delta_{\rm f}}{\lambda_{\rm f}}$$

while the influence of $R_{\text{th, f}}$ is insignificant compared with that of the thermal resistance of contiguous materials [47]. Nevertheless, bearing in mind falling values of thermal conductivity with decreasing nanofilm thickness, thermal resistance of the film may to a certain extent (depending on the number of atomic layers) influence total thermal resistance of the entire system. Moreover, the film has at least one interface with the solid on which the phonon scattering takes place.

Electrons transferring heat in a metal or semiconductor cause lattice vibrations leading to the predominant formation of optical phonons converted into high-frequency acoustic ones during their motion in the material. Scattering of longitudinal optical phonons at the interface gives rise to a transverse constituent that complicates the scattering pattern. The effect of a material border on phonon propagation is a critical factor exerting a decisive influence on thermal conductivity in nanosystems.

The spatial region of maximally intensive formation of optical phonons adjoins the border of a material from which the heat is withdrawn. The characteristic size *r* of the region in which optical phonons are formed is comparable to the lattice size; it is much smaller than the phonon mean free path $(l \approx 250 \text{ nm})$. This distinction is another critical factor responsible for higher real temperatures in the border area compared with those calculated from the diffusion theory, the difference between real and calculated temperatures increasing in direct proportion to l/r.

The third critical factor is related to the fact that the group velocity of the optical phonons being formed is significantly lower than the characteristic lattice thermal conductivity rate, which accounts for the elevated concentration of these phonons in the zone of their active formation [67]. The increase in phonon concentration near the 'cold' border of the material gives rise to the negative phonon flow responsible for additional thermal resistance close to the border.

The thickness of a nanofilm can be either greater or smaller than the phonon mean free path. As the film thickness decreases and becomes commensurate with the lattice size, the excess temperature at the heat-releasing interface, caused by the second and third critical factors, also falls. Simultaneously, the role of scattering from the interface (first critical factor) increases. While longitudinal thermal conductivity of the film in the direction normal to the interface decreases, its constituent along the interface may grow due to the appearance of the transverse component of the phonon wave vector during scattering; it may be greater than the longitudinal one.

Enhancement of thermal conductivity along the filmsolid interface is attributed to the properties of one- and two-dimensional nanostructures characterized by specific surface phonon propagation patterns. Experiments with one-dimensional carbon nanotubes having a thickness from a few nanometers to several dozen nanometers showed that such systems have a thermal conductivity of about $3000 \text{ W} (\text{m K})^{-1}$ at room temperature and transfer heat flux with minimal losses, just as superconductors and optical waveguides transfer electric current and light, respectively. Surface thermal conductivity decreases with decreasing temperature and becomes a few orders of magnitude lower $[0.1-1 \text{ W} (\text{m K}^{-1})]$ at temperatures close to absolute zero than at room temperature. A quantum of phonon thermal conductance in one-dimensional nanostructures can be calculated as [cf. formula (29)] [67]

$$\alpha_{\rm ph,\,min} = \frac{\pi^2 k^2 T}{3h} = \frac{\pi k^2 T}{6\hbar} \,. \tag{31}$$

It can be seen that $\alpha_{\text{ph},\,\text{min}}$ grows linearly with temperature.

Nanofilms exhibit two-dimensional thermal conductivity, but the principles of heat transfer by surface phonons remain unaltered, which accounts for the appearance of the transverse component of the wave vector during scattering from the interface.

Nanofilms form a subgroup in a wider group of nanomaterials containing amorphous or vitreous substances, materials with nano-sized grains and nanopores, multilayer films, and epitaxial lattices. A common distinctive feature of these nanomaterials is the possibility of identifying an elementary nanostructure and reproducing it to obtain any necessary amount of a given material. The size of an elementary nanostructure in amorphous materials is close to the lattice size. Multilayer films have a period depending on the thickness of the elementary structure which may consist of two layers of alternating materials. The thermal conduction in nanomaterials is characterized by the presence of collective modes and phonon interference.

Amorphous and porous materials possess a low permittivity, associated with low thermal conduction. Nanofilms of such materials widely used in electronics need efficacious cooling. By way of example, modern electronic logical units consist of several metallic (Cu) layers alternating with dielectric (polyamide) films less than 500 nm in thickness. The number of layers is increasing and their thickness decreasing with advances in technology. As a result, such nanostructures as multilayer films and superlattices have become available.

Multilayer nanostructures are systems composed of alternating layers of different materials as thick as a few nanometers to several hundred nanometers. Multilayer films consist of amorphous or polycrystalline materials, while superlattices are single-crystalline structures. Multilayer nanosystems exhibit two characteristic examples of thermal conduction in which phonon mean free path is either smaller or larger than the period defined as the thickness of an elementary nanostructure composed of two or more layers.

As shown in experiment, the former type of thermal conduction shows weak dependence on the thickness, i.e., phonons with the mean free path close to the film thickness have little effect on heat transfer.

The thermal resistance of a multilayer system is calculated as the sum of resistances of the constituent films and interfaces. In the case of amorphous films, thermal resistances of the interfaces are, as a rule, low compared with layer resistance. Therefore, thermal conductance of a multilayer film is practically independent of the period. The weak influence of interface resistances was confirmed experimentally for such contact pairs as Y_2O_3 –SiO₂, and ZrO₂– Y_2O_3 [67].

The second type of thermal conductance is inherent in superlattices. If the phonon mean free path is 10 times or more larger than the period, the interference of waves reflected from different interfaces leads to discontinuities of phonon frequency distributions due to:

— a substantial decrease in the group velocities of phonons, especially high-energy acoustic ones;

— an increase in the number of scattering and umklapp processes.

If the phonon mean free path is not sufficiently long so as to cause discontinuity of frequency distribution, the effects of a single interface become the main factor responsible for thermal resistance in the superlattice; these effects arise from:

— different scattering patterns in contacting materials;

- defects and dislocations in materials with different lattice constants;

- surface roughness;

- diffusion and fusion of materials.

Moreover, thermal resistance of multilayer systems is influenced by the lattice period and the temperature dependence of thermal conductivity of the materials. Experiments with Si–Ge contact pair superlattices showed that the thermal conductivity of a material decreases with decreasing the layer thickness if it is much smaller than the critical one. An increase in the lattice period, as a rule, leads to a rise in thermal conductivity, provided the film thickness does not exceed the threshold value at which surface defects begin to manifest themselves and lower the thermal conductivity. When the lattice period is greater than the film critical thickness equaling the phonon mean free path, its further growth does not cause an additional rise in thermal conductivity, and thermal conductance of the lattice largely depends on the number and resistances of the interfaces.

Surface roughness of superlattice layers is usually small. However, the effect of surface properties may be enhanced by physical and chemical processes when growing one material on the surface of another. Also possible is asymmetric formation of interfaces due to the difference between residual events during the growth of material A on the surface of material B, and material B on the surface of A.

As interface density (the number of contacts per lattice thickness) increases, thermal conductivity of the lattice made from A-B materials approaches that of the corresponding AB alloy. It may be either higher or lower than alloy thermal conductivity. It is supposed that the key factor in this case is the difference between acoustic impedances of materials A and B: the greater it is, the lower the lattice thermal conductivity. Heat flux directionality may also play a certain role.

The following main approaches are applied to the theoretical description of thermal conduction in superlattices [67]:

- consideration of phonons as heat waves;

— representation of phonons as particles transferring elementary thermal perturbations with the use of the Boltzmann equation;

- numerical simulation based on molecular dynamics methods.

The theory of multilayer films is incomplete. Many of its provisions need experimental verification, while a wealth of experimental data await theoretical interpretation. Suffice it to mention the lack of experimental observations reliably confirming the prediction of discontinuities in phonon frequency distributions. On the other hand, there are no theoretical models for the evaluation of interface density effects on lattice thermal conductivity that may be either higher or lower than that of the corresponding alloy. Such models must ensure the possibility of describing the lattice properties in alloys with different acoustic impedances that are equally poorly studied in experiment.

For all that, the available data on thermal conduction in nanofilms allow for the following conclusions [67]:

— the thermal resistance of interfaces essentially manifests itself at an acoustic impedance ratio of the lattice contact pair higher than 1.1;

— the difference between acoustic impedances leads to a rise in the reflection coefficient of incoherent phonons and to the appearance of discontinuity in the frequency spectrum of coherent phonons whose group velocity decreases;

— phonons from different parts of a given frequency spectrum are scattered differently: propagation of highfrequency phonons with wavelengths on the order of several atomic layers is hampered by the scattering characteristic of alloys, while that of low-frequency phonons with greater wavelengths is hampered by scattering typical of multilayer films;

— the thermal resistance of interfaces depends on surface roughness, diffusion, and residual properties of physical and chemical transformations during the growth of one material at the surface of another, heat flux directionality, and temperature;

— the phonon thermal conductivity of a superlattice may be either higher or lower than that of the corresponding alloy and tends to it as interface density increases.

It is predicted that heat flux propagation parallel to interfaces should be accompanied by a rise in thermal conductivity compared with that of an alloy due to formation of surface modes. At the same time, measurements of this constituent in GaAs–AlAs superlattices revealed an approximately fourfold decrease in thermal conductivity relative to its values in materials of contact pairs.

Very few theoretical works treat nanofilm thermal conductivity as a consequence of electron–phonon interaction. Studies conducted in the framework of the local temperature concept have demonstrated a wide dispersion of results depending on the conditions at interfaces between materials.

8. Conclusions

From the standpoint of irreversible thermodynamics, resistance *R* is a parameter defined by the ratio of potential difference $\Delta \varphi_X$ of the physical quantity *X* to the flux Φ_X of a given quantity:

$$R = \frac{\Delta \varphi_X}{\Phi_X}$$

In the case of thermal resistance, the role of a heat flux potential is played by temperature, and temperature difference ΔT in the numerator corresponds to the heat flux Q in the denominator [absolute thermal resistance (2)]. Replacement of the heat flux by its density q turns thermal resistance into a specific one (1) that characterizes the thermal properties of a unit area of cross section or of a surface of the material. Because specific thermal resistance is unrelated to the quantitative characteristics of materials, it is a thermodynamically intense quantity depending only on the properties of a given material. In contrast, absolute thermal resistance is an area-dependent thermodynamically extensive quantity.

When considering contact phenomena to determine thermal resistance, the potential difference between interacting surfaces is used along with the heat flux across the contact zone. Thermal contact resistance is a variable depending on many factors, which accounts for the nonlinearity of thermal processes in the contact zone and the impossibility of flux– potential interrelation via constant coefficients. This problem can be addressed in two ways:

- presentation of contact resistance as a function of parameters that influence it:

$$R=f(x_1,x_2,\ldots,x_n);$$

— disuse of the notion of 'contact resistance' and establishment of a direct relation between the flux and the potential of a physical quantity in the form

$$\Phi_X = f(\Delta \varphi_X),$$

as in the diode theory for obtaining relationships of the type

j = f(U).

The former approach is preferred when applying to real joints.

The thermal contact theory closely resembles the Holm theory distinguishing the main components of electrical contact resistance and describing their influence on electron emission and tunneling across the contact zone. Also, the constituents of thermal contact resistance also have analogs in electrical resistance. In other respects, these theories differ. Suffice it to say that components of contact electrical resistance are analyzed by quantum-mechanical methods due to the explicit discreteness of electric current carriers, while constituents of thermal contact resistance are calculated relying on continuous medium methods; this necessitates the introduction of fictitious thermal conductivity and empirical coefficients.

Thermodynamic interpretation of thermal resistance makes possible the determination of its limiting values in respect to a contact. Specific contact resistance is an intensive quantity characterizing the individual properties of materials. For this reason, specific constriction resistance is convenient to find as the thermal conduction resistance of a flat wall thermally equivalent to the perturbed zone. The wall area is assumed to equal the real contact area. The specific resistance of the wall being unrelated to its area, it confirms the intensive character of the properties of specific constriction resistance identical for both a single microcontact and the entire macrocontact. An adiabatically isolated material with a zero real contact area possesses no additional thermal resistance besides intrinsic thermal conduction resistance. From this it is apparent that specific constriction resistance serially introduced into the thermal scheme of a joint together with resistances for thermal conduction of the materials should vanish in the absence of a real contact area. Because specific constriction resistance also tends to zero as the real contact area approaches the nominal value, it has a maximum at the real-to-nominal area ratio of 0.201. Total constriction resistance depends on the joint area, i.e., it is a thermodynamically extensive quantity with the following limits: it vanishes when the relative real contact area is equal to unity, and tends to infinity at a zero value of this area. In a system with specific constriction resistance boundaries, these values correspond to the limits of expressions (4), (5).

The following problems remain to be finalized in the thermal conduction theory:

— calculation of thermal resistance in intimate contacts reported to have a finite value in experiment [37], in conflict with the boundary condition of the fourth kind;

— experimental justification of the extremum of perturbation zone thickness and the thermal contact resistance limit in the region of low contact pressures;

— application of equivalent models of the perturbation zone, based on fictitious parameters of thermal conductivity and capacity, to nonstationary processes with a characteristic time below the microconstriction time; - evaluation of thermal contact resistance taking account of electronic and radiative constituents.

Nanoscale devices and materials are extensively used in modern technologies. Experimental studies have demonstrated that thermophysical processes at nanometer scales are essentially different from analogous processes in macroand microstructures. Application of up-to-date methods of molecular dynamics and quantum mechanics to the computation of thermal processes in nanosystems permitted simulating the experimentally examined increase in the temperature gradient in ideal contacts of crystals and calculating their related thermal resistance. Moreover, new conclusions were drawn concerning the dependence of the ideal contact transition coefficient on phonon frequency. Experimental data and mathematical models for their description need novel physical interpretations. This goal can be achieved by resolving such fundamental problems as the determination of temperature in systems smaller than the Casimir boundary and elucidation of heat transfer mechanisms in systems with the phonon mean free path smaller than the lattice constant. Further studies are needed on thermal interactions between materials with different dielectric properties, including heat flux propagation in metal-semiconductor and metal-dielectric contacts where electron thermal conductivity is converted into phonon thermal conductivity or splits into several constituents.

The solution to these problems is hampered by the imperfections of the thermal devices, such as poor accuracy and a large time constant of heat flux sensors (the flux value must be known to calculate thermal contact resistance). An important tool for contact heat exchange studies is provided by the recently developed bismuth-based gradient heat-flux sensors with a time constant of $\sim 10^{-8} - 10^{-9}$ s and relative error of 2-3% using the transverse Seebeck effect [71]. The feasibility of direct graduation of thermal e.m.f. with respect to heat flux density was demonstrated for Al-Si contacts at low temperatures [30, 72, 73]. The use of sensors based on metal-semiconductor contacts opens good prospects for the evaluation of time constants and sensor accuracy, bearing in mind that only a few types of currently available sensors are suitable for reliably measuring heat fluxes at cryogenic temperatures.

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