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Quantum phonon transport in 3D metal–dielectric point polycontacts with strong lattice distortions

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The experimental results and theoretical analysis of the heat flux in an Si–Cu pressure-made 3D point contact are given. The contributions of the quantum phonon transport, weak electron–phonon interaction and strong phonon-lattice distortion scattering to the phonon heat flux are theoretically investigated.

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66.70.+f Nonelectronic thermal conduction and heat-pulse propagation in solids; thermal waves (for thermal conduction in metals and alloys);
68.35.Ja Surface and interface dynamics and vibrations ... Solid-solid interfaces: transport and optical properties.

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1. Introduction

The point contact (PC) is a unique physical device that makes it possible to realize a hightly nonequilibrium state of electron or phonon systems (see reviews [1,2]). Heat transport in metal–dielectric PCs is realized by practically noninteracting groups of phonons coming from the opposite edges of the PC. Near the junction an equilibrium temperature cannot be reached, and the fluxes there cannot be calculated in terms of the thermodynamics of nonequilibrium processes.

At present it has been established that quantum phonon transport is realized for the three-dimensional (3D) metallic point contact. The fabrication of such contacts permits one to study the quantized electron–phonon system in a nonlinear thermal regime. The Landauer–Buttiker formalism [3,4] may be used to calculate the quantum phonon flux in a point contact, and the extension of this formalism takes into consideration also the temperature jump near the PC [5].

Experiments on the thermal conductivity of metal–insulator 3D point contacts reveal an anomalously large peak of the reduced phonon heat flux in the interval 0.1–10 K [6,7]. This effect can be attributed to the quantum «diffractional blocking» of phonons. The theory of quantum phonon transport was developed for 3D PC [8] and 2D microbridges [9–12]. Quantum phonon transport was measured in experiments on a mesoscopic suspended 2D beam [13]. In this paper we show that phonon scattering in a 3D pressure-made PC may mask the details of the quantum phonon transport regime.

2. Experimental procedure

The phonon heat transport was measured for a silicon crystal at temperatures in the range from 0.1 to 10 K, using the anvil-needle technique. Point contacts were made by mounting a rectangular Si single crystal on three sharp tips. One of the tips was made of Cu (OFHC), and two others were made of Vespel polymer resin (the thermal conductivity of Vespel resin below 10 K is very low). The Cu tip was etched shortly before the PC was formed. A neutron transmutation doped natural Ge crystal was mounted on the Si as a thermometer; the leads were 50 μm diameter superconducting leads. The flat surfaces of the Si were cut with a diamond saw. The average surface roughness was about 2 nm for polished surfaces. The measurement technique is described elsewhere [2]. The

heat flux curves were measured below 10 K. The temperature of the Cu needle was kept at $T_0 < 0.1$ K. The heat flux was determined from the known heat capacity of silicon and the time dependence of the Si crystal temperature. For Si–Cu PCs, substituting the cold edge with a Cu needle makes it possible to obtain stable metal–dielectric contacts 10–100 nm in size. For such PCs the phonon–electron scattering contribution is negligibly small [2] for Si crystal temperature (T) in the range $0 < T < 10$ K. After the heater was switched off, the cooling curve of the Si sample was measured, i.e. the temperature dependence $T(t)$ was found, and the derivative dT/dt as a function of T was found by numerical differentiation. Using the thermodynamic definition of the heat capacity the heat flux $\dot{Q}(T)$ can be calculated from the equation:

$$\dot{Q} = C(T)\left(\frac{dT}{dt}\right), \qquad (1)$$

where $C(T)$ is the heat capacity of the Si sample at temperature T. We neglect the opposite heat flux from the Cu needle.

3. Model of single ballistic point contact

Dimensional transport effects appear as the dimensions of nanostructures decrease. These effects are associated with the ratio between the geometric characteristics of the structures and the scattering lengths corresponding to various carrier scattering mechanisms. Ballistic charge and heat transport intensifies in PCs at low temperatures for values of the contact diameter ranging from 10 nm to 1000 nm. Under these conditions the inelastic scattering lengths of charge and heat carriers become large compared with the dimensions of the contact. When the contact dimensions drop below 10 nm, size-quantization of phonons in the contact appears. Heat is transported in a ballistic PC by two noninteracting groups of phonons, whose distribution functions are given by the temperatures of the bulk edges of the contact T and T_0 [5]:

$$\dot{Q}_B(T,T_0) = \frac{\hbar S_0}{2(2\pi)^3} \times$$
$$\times \sum_{\alpha} \int d\mathbf{k}\, \omega^{\alpha}(\mathbf{k})\, u_z^{\alpha} D_{1,2}^{\alpha} \{N(\omega^{\alpha},T) - N(\omega^{\alpha},T_0)\}. \qquad (2)$$

Here S_0 is the area of the contact, $\omega(\mathbf{k})$ is the phonon dispersion law, $\boldsymbol{u}^{\alpha} = \partial\omega^{\alpha}(\mathbf{k})/\partial\mathbf{k}$, $\mathbf{k}$ is the wave vector of a phonon, and α is the index indicating the branch of the phonon spectrum. If the phonon distribution functions in the bulk edges are equilibrium functions, then

$$N = n_p(\omega,T) = \left[\exp\left(\frac{\hbar\omega}{T}\right) - 1\right]^{-1}. \qquad (3)$$

The expression (2) contains the coefficient of the phonon energy transfer $D_{1,2}^{\alpha}(\mathbf{k})$ from edge 1 to edge 2; the dispersion law is taken into account for edge 1. The magnitude of the heat flux remains unchanged if the corresponding quantities for edge 2 are used in Eq. (2). This is a consequence of the reciprocity theorem for the transmission of elastic waves through an ideal interface [14].

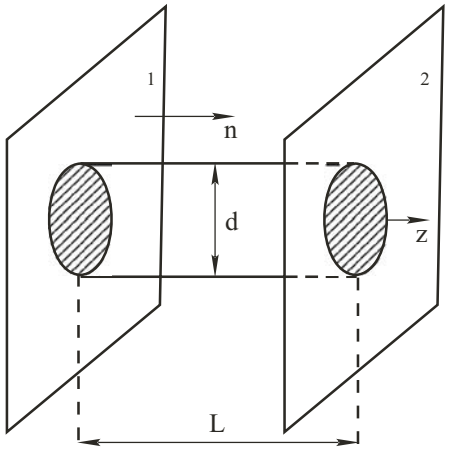

Fig. 1. Diagram of a point contact in the form of a cylindrical short-circuit in a vacuum gap between the surfaces Σ_1 and Σ_2.

A form of the energy transfer coefficient used for quantum flux calculation is the «spherical flow» model for the geometry of the contact [15]. This model can be obtained by rolling the initially flat surface of the screen into a tube and gluing the edges of the contact on the surface of a sphere. For a wave incident along the z axis the solution of the wave equation is symmetric with respect to this axis, and the Neumann condition is satisfied on the surface of the contact, rolled into a tube of vanishingly small diameter, as a result of the cylindrical symmetry (see Fig. 1).

4. Model of polycontact

We calculated the point-contact heat flow carried by phonons in an Si–Cu pressure-made PC. It is necessary to take account of the fact that the surface of a contact, as a rule, consists of a collection of separate microscopic con-

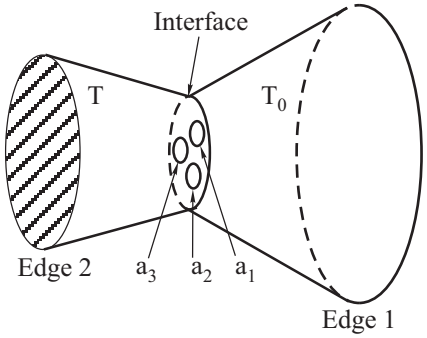

Fig. 2. Schematic model of a contact: T and T_0 are temperatures of the massive edges of the contact; a_1, a_2 and a_3 are zones with different microscopic contacts.

tacts (MCs). Therefore the total phonon flux through the contact is a sum of the fluxes through individual MCs.

We denote the separate point contact as a microscopic contact (see Fig. 2).

5. Computation of heat flux

The combination of quantum phonon transport in a such polycontact geometry and diffusive phonon scattering in the Si near-contact region can be represented by equations for the heat flux:

$$\dot{Q}(T,T_0) = \frac{\hbar A_G}{(2\pi)^3}\int d\omega\ \omega D_{\text{Si–Cu}} S(\omega)\times$$

$$\times K(l_{\text{Si}},\omega)[N_p(\omega,T)-N_p(\omega,T_0)]\ , \qquad (4)$$

where:

$$K = \frac{32}{3\pi}D(\omega)\frac{l_{\text{Si}}}{d_G}\left(D(\omega)+\frac{32}{3\pi}\frac{A_G}{A_{\text{MICRO}}}\frac{l_{\text{Si}}}{d_G}\right)^{-1}. \qquad (5)$$

Here, A_G is the general area of point contact, A_{MICRO} is the sum of MCs areas, $D_{\text{Si–Cu}}$ is the coefficient of Si–Cu acoustic mismatch, $D(\omega)$ is the coefficient of quantum phonon energy transport for separate MC [1–3], $S(\omega)$ is the spectral function of Si lattice [9], d_G is the diameter of the polycontact region, and l_{Si} is the effective phonon scattering length for the near-contact region for Si. We omit the sum over the phonon spectrum branches. For the case of the linear phonon dispersion law it follows that

$$S(\omega) = \pi\omega^2 u_{\text{Si}}^{-2}\ . \qquad (6)$$

Here u_{Si} is the group velocity for Si. We represent $D(\omega)$ as the sum over normal modes, numbered by n, of the acoustic wave transmission through separate MCs:

$$D(\omega) = 4\pi A_0 u_{\text{Si}}^2 \omega^{-2}\Phi(\omega)\,, \qquad (7)$$

$$\Phi(\omega) = \sum_{n=0}^{\infty}(2n+1)T_n\,(d_0 u_{\text{Si}}^{-1}\omega)\,. \qquad (8)$$

Here d_0 is the diameter of a separate MC and T_n is the transmission coefficient of nth normal mode. For $n > 0$, the functions $T_n(x)$ are in the form of jagged steps: $T_n(x) = 1$ for the frequencies at which the normal quantum mode with number n begins to pass through the MCs. In Ref. 8, the calculation of T_n is discussed for the case of a 3D channel with rigid surface.

6. Experimental results

Measurements for a Si–Cu PC reveal well defined quantum diffraction blocking in the range from 0.1 to 0.8 K, and the reduction of the reduced heat flux in the range from 1 to 10 K (see Fig. 3).

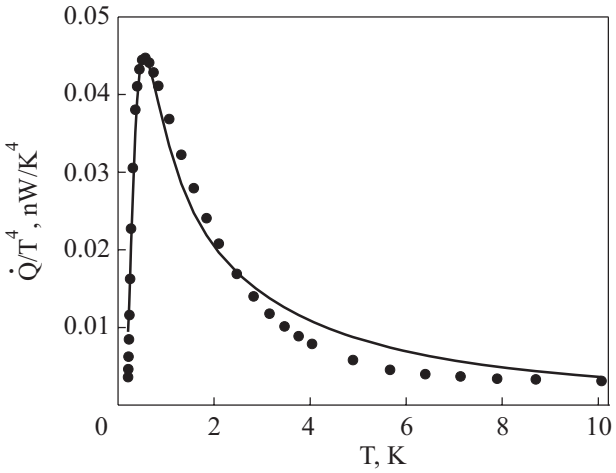

Fig. 3. Reduced heat flux $\dot{Q}/T^4$ through Si–Cu point contact. (●) is the experimental data, solid line is theoretical calculation by Eqs. (4)–(9).

The theoretical analysis reveals the polycontact structure and the characteristics of subsurface lattice distortions. We introduced scattering length as

$$l_{\text{Si}}(T) = l_D\left(\frac{\theta_D}{T}\right)^s. \qquad (9)$$

In our experiments s varies in the range $1.2 < s < 1.6$. Such a weak temperature dependence (compared to the Rayleigh phonon scattering) is typical for phonon scattering due to statistical strain fields of dislocations [16].

The results of the heat flux computation are in good agreement with experimental data for a 7 g silicon single crystal in the whole temperature interval of the measurement. The best fit to the experimental data is for $T_0 = 0.1$ K, $L = 120$, $d = 32$, $A_{\text{MICRO}}/A_G = 1$, $d_G = 10^5$ nm, $l_D/d_G = 5.03\cdot10^{-5}$, $S = 1.4$ (Fig. 3). The estimates from calculations are $d_0 = 20$ nm for the diameter of each separate microscopic contact and 50 nm for its effective length. The last parameter shows the typical scale of subsurface lattice distortions. The enhancement in the heat flux reported here at a temperature where the dominant phonon wavelength is of the order of a typical point contact dimension demonstrates the wave nature of phonons.

7. Discussion

The Si–Cu point contact was made by the anvil-needle technique, and the emergence of the stress fields in the contact region seems natural.

The electronic system in metal–dielectric point contacts makes a small contribution to the heat transport process as long as the size d of the point contact remains small compared with the effective phonon–electron scattering length l_a [2]. For ballistic phonon transport l_a

equals the phonon–electron scattering length $l_{\text{ph-}e}$ in a pure metal. For strong elastic scattering l_a depends on the relaxation length l_r of phonons over quasimomentum, $l_a = (l_{\text{ph-}e} l_r)^{1/2}$. Apparently, when diffraction effects are taken into account in phonon transport in point contacts, the picture becomes more complicated than in the case of electron transport. This is because the boundary conditions for elastic waves on the surface of a contact are more complicated. For real contacts these conditions may not reduce to the Neumann and Dirichlet problems stated here. A discussion of the choice of boundary conditions in quantum-mechanical problems can be found in Ref. 17. The polycontact structure of pressure-made PCs was studied using an alternative method in [18].

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