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On the Influence of Tunneling on the Efficiency of Thermoelectric Devices

It is known that the efficiency of thermoelectric materials is determined by the Ioffe parameter $Z = \alpha^2\sigma/\chi$, where α is the thermoelectric emf, σ the conductivity, and χ the thermal conductivity. The latter is the sum of the lattice thermal conductivity χ_L and that of the electron (or hole) gas χ_e. For a given scattering mechanism, the quantity χ_e is proportional to σ, and hence it has become impossible to gain in efficiency by reducing it. At the same time, the quantity χ_L is associated with parasitic dissipation processes, and the obvious way to increase efficiency consists in lowering the lattice thermal conductivity. A. F. Ioffe proposed, as one of the ways of increasing Z, introducing into the crystal such impurities as would effectively scatter phonons but be only weakly reflected in the motion of the carriers. In particular, this can be achieved by creating disordered alloys ([1]).

In the present work another possible way of increasing σ/χ is considered: the use of microscopic discontinuities in the continuity of the crystalline medium. The simplest example of such defects is a microscopically narrow slit between two pieces of one and the same material. It may be expected that such defects will affect the transmission of phonons more strongly than that of electrons. Indeed, the radius of interatomic forces is small, and for a slit width of several lattice constants the phonon coupling between the two pieces proves to be practically broken. At the same time, electrons can pass through the slit either over the barrier or by means of thermoelectronic emission. In particular, in the limiting case of a sufficiently wide slit, conditions are obtained that are typical of a vacuum thermoelectronic converter, where, as is known, heat transfer by the lattice is entirely absent.

We shall be interested, however, in the case of smaller distances, when electron passage through the slit occurs over the barrier. Unfortunately, there is no way to estimate the transmission coefficient reliably from purely theoretical considerations, and it will enter as a phenomenological parameter. To estimate the effect from above, it is assumed that lattice thermal conductivity through the slit is entirely absent. At high degrees of doping, heat transfer by radiation

Fig. 1. Illustration of the band diagram near a vacuum tunnel gap

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does not occur.

The charge and energy fluxes through the slit between two semi-infinite plates are given by the expressions:

$$I = -\frac{em^* D}{2\pi^2 \hbar^3} \int_0^\infty \varepsilon \left[f_c(\varepsilon) - f_h(\varepsilon) \right] d\varepsilon, \tag{1}$$

$$W = \frac{m^* D}{2\pi^2 \hbar^3} \int_0^\infty \varepsilon^2 \left[f_c(\varepsilon) - f_h(\varepsilon) \right] d\varepsilon. \tag{2}$$

Here D is the transmission coefficient (its dependence on energy for electrons near the bottom of the conduction band may be disregarded); m^* is the effective electron mass; $f(\varepsilon)$ is the Fermi distribution function–

tion. In doing so, it is borne in mind that, according to (2), the contribution of the nonequilibrium part of the distribution function to the fluxes is small. It is assumed that between the points c (cold) and h (hot) at the edges of the gap there exists a potential difference U_{ch}, with $U_{ch} = -U_{hc}$, so that (see Fig. 1)

$$f_c(\varepsilon) = f(\varepsilon - \mu_c / kT_c), \qquad f_h(\varepsilon) = f((\varepsilon - \mu_c - eU_{ch})/kT_h). \tag{3}$$

The expressions for the fluxes in the continuous regions have the form

$$j = \sigma E_i - \alpha\sigma(\Delta T)_i, \quad i = \mathrm{I}, \mathrm{II}; \qquad W = (\Phi_\gamma + \alpha T_\gamma) j - \varkappa(\nabla T)_i, \quad \gamma = c, h. \tag{4}$$

For given temperature values at the outer ends of the plates T_1 and T_2 and current j, the system of equations (1), (2), (4) makes it possible to determine completely the temperature and electric fields in the system. In this case, of course, it is meaningless to speak of the Peltier effect at the edges of the gap, since the space inside the gap cannot be regarded as a separate phase. All thermal effects are taken into account automatically, since the balance equation is written for energy, not heat.

Fig. 1. Illustration of the band diagram near a vacuum tunnel gap

The first estimates of the electrical and thermal conductivities of a vacuum gap can be obtained using only equations (1) and (2). The electrical conductivity of a unit area of the vacuum gap is calculated for $T_h - T_c = 0$ and $U_{hc} \to 0$ and is equal to

$$\sigma_S = \frac{De^2 m^* kT}{2\pi^2 \hbar^3} F_0(\eta). \tag{5}$$

A similar result was obtained in ([2]).

The expression for the thermal conductivity of a unit area of the vacuum gap, obtained for $j = 0$ and $T_h - T_c \to 0$, has the form:

$$\varkappa_S = \frac{Dm^* k^3 T^2}{2\pi^2 \hbar^3} \left[6F_2(\eta) - \frac{4F_1(\eta)}{F_0(\eta)} \right]. \tag{6}$$

Here the following notation has been adopted: $\eta = \mu/kT$ is the reduced chemical potential; $F_p(\eta)$ $(p = 0, 1, 2)$ is the Fermi integral of index p. The values of σ_S/D and $\varkappa_S/D$, calculated at 300° K, are given in Table 1.

It is interesting to note that for transfer through the gap one can introduce an analogue of the Lorenz number, namely,

$$\frac{\varkappa_S}{\sigma_S} = LT;$$

$$L = \frac{[6F_2(\eta) - 4F_1(\eta)/F_0(\eta)]}{F_0(\eta)} \left(\frac{k}{e}\right)^2. \tag{7}$$

Table 1

Numerical values of the quantities σ_S/D and $\varkappa_S/D$

η	$\frac{\sigma_S}{D}$, $\frac{1}{\Omega \cdot \text{cm}^2}$	$\frac{\varkappa_S}{D}$, $\frac{\text{W}}{\text{deg} \cdot \text{cm}^2}$
−4	$7.75 \cdot 10^5$	3.66
−2	$5.43 \cdot 10^6$	$2.47 \cdot 10^1$
0	$2.97 \cdot 10^7$	$1.44 \cdot 10^2$
2	$9.1 \cdot 10^7$	$5.3 \cdot 10^2$
4	$1.71 \cdot 10^8$	$1.03 \cdot 10^3$
6	$2.54 \cdot 10^8$	$1.95 \cdot 10^3$
8	$3.43 \cdot 10^8$	$2.2 \cdot 10^3$
10	$4.3 \cdot 10^8$	$3.16 \cdot 10^3$

The multiplier in front of $(k/e)^2$ varies from 2 at $\eta = -4$ to 3 at $\eta = 10$, i.e., as the degree of degeneracy increases it approaches its standard value $\pi^2/3$.

Of great interest are the effective characteristics of porous-type substances, in which the case of a vacuum gap is realized. It is easy to see that, for a model of a substance consisting of elementary cells in the form of rectangular bars of length

l with a gap, the effective values of the electrical and thermal conductivities are expressed as follows:

$$\sigma_{\text{eff}} \cong \frac{l}{l/\sigma + 1/\sigma_S}; \qquad \varkappa_{\text{eff}} \cong \frac{l}{l/\varkappa + 1/\varkappa_S}. \tag{8}$$

It is easy to derive formulas for models with an arbitrary geometry of the "elementary cells."

In the case $j = 0$, solving the system (1), (2), (4) in the linear approximation with respect to $(T_h - T_c)/T_h$ leads to the following results.

The potential difference arising across the vacuum gap is related to the temperature difference across it by the relation

$$-eU_{ch}/k(T_h - T_c) = [2F_1(\eta)/F_0(\eta) - \eta] \equiv K(\eta). \tag{9}$$

Figure 2 shows the dependence $K(\eta)$. The effective integral characteristics of an elementary block with a gap are expressed as

$$\frac{\alpha_{\text{eff}}}{\alpha} = 1 - \left[1 - \frac{k}{e}\frac{K(\eta)}{\alpha}\right]\frac{T_h - T_c}{T_2 - T_1}; \tag{10}$$

$$\frac{\chi_{\text{eff}}}{\chi} = \frac{2(T_2 - T_h)}{T_2 - T_1}. \tag{11}$$

The calculation, carried out under the condition that the carrier concentration in the solid does not depend on temperature, for a specimen of size 2 cm for var $T_1 = 300$–900°K and var $T_2 = 400$–1000°K, did not reveal nonlinearity in the temperature dependence of χ_{eff}. Note that, according to (2), at small currents no nonlinearity is observed in the electrical conductivity either.

Also of interest is the fundamental possibility of a gain in α_{eff}, which follows from (10). Indeed, under the condition

$$\left|\frac{k}{e}\left[\frac{2F_1(\eta)}{F_0(\eta)} - \eta\right]\right| > |\alpha| \tag{12}$$

the inequality $\alpha_{\text{eff}}/\alpha > 1$ proves to be satisfied. For nondegenerate semiconductors with a simple band structure, the relation

$$\alpha = \frac{k}{e}\left(r + {}^5/_2 - \eta\right) \tag{13}$$

holds.

Fig. 2. Dependence of K on η

Figure 2: Fig. 2. Dependence of K on η

Fig. 2. Dependence of K on η

For scattering by phonons $r = -{}^1/_2$; for scattering by impurity ions $r = {}^3/_2$ (3).

From comparison of (12) and (13) it follows that a gain in thermoe.m.f. will be observed for scattering by phonons at $\eta > -4$, and for scattering by impurity ions at $\eta > 3$.

Thus, even simple estimates carry interesting information about possible tendencies in the change of the properties of substances with microgaps and microdefects. Of course, the present work should be regarded only as a first attempt to clarify such tendencies, and it is still too early to speak of comparison with experiment; however, such a comparison for specific models is expected to be carried out in the near future.

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Note: Figure translations are in progress. See original paper for figures.