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MISCELLANEOUS

INFLUENCE OF THE CONCENTRATION DISTRIBUTION OF WEAKLY DEGENERATE CARRIERS ON THE EFFICIENCY OF AN ARM OF A THERMOCOUPLE

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The one-dimensional boundary problem on determination of a stationary temperature field in an adiabatically isolated one-dimensional arm of a thermocouple has been numerically solved. Calculations were carried out for two regimes of operation of the thermocouple, one which was characterized by a maximum temperature drop and the other by a maximum refrigerating capacity. The method of quantum statistics of carriers was used in the calculations. Homogeneous and inhomogeneous arms with different carrier-concentration distributions were considered. It is shown that a linear distribution cannot be considered as optimum.

The insufficiently high efficiency of thermoelectric coolers limits their use in practice; therefore, upgrading the quality of thermoelectric conductors is one of the most important problems of their physics. At present, there are no reliable methods of optimizing these conductors; this being so, their potentialities are not used completely. The use of thermoelectric conductors in coolers is determined by the operating conditions and temperatures for which they are designed; therefore, it is necessary improve the properties of a thermoelectric conductor in a definite temperature range. This problem can be solved by different methods. In the present work, we propose a method of upgrading the quality of a thermoelectric conductor in the operating-temperature range of a thermocouple.

A thermoelectric conductor is usually optimized by its thermoelectric-quality coefficient Z [1], determined as

$$Z = \frac{\alpha^2 \sigma}{\chi} . \quad (1)$$

The dependence of the value of Z on the temperature and the characteristics of the charge carriers in a conductor is usually determined without regard for the lattice component or the electronic component of heat conduction. In the latter case, the kinetic effects proceeding with the participation of nongenerate carriers are defined by comparatively simple analytical expressions and, therefore, the thermoelectric quality of a conductor can be calculated practically completely [1]. However, these calculations give an approximate value of Z because the charge carriers in thermoelectric conductors are somewhat degenerate in the range of their maximum efficiency [2].

Moreover, it is well to bear in mind that the thermoelectric-quality coefficient is introduced to characterize the temperature-independent kinetic effects [1] occurring in a conductor and cannot be considered as a reliable characteristic of variable processes. Therefore, to determine the efficiency of an arm of a thermocouple, we will calculate the temperature drop in it. The temperature field of an adiabatically isolated, homogeneous, one-dimensional arm of a thermocouple operating in a stable regime is defined, with allowance for the Thomson effect, by the stationary heat-conduction equation

$$\frac{d}{dx}\left(\chi \frac{dT}{dx}\right) + \frac{y^2}{\sigma} - yT \frac{d\alpha}{dT} \frac{dT}{dx} = 0 \quad (2)$$

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with boundary conditions

$$\chi \left.\frac{dT}{dx}\right|_{x=0} = \alpha y T\big|_{x=0} - q_0\,, \quad T\big|_{x=1} = T_1\,. \tag{3}$$

Since, even in strongly doped semiconductors at liquid-nitrogen temperature and higher temperatures, charge carriers are predominantly scattered by vibrations of the crystal lattice, we will restrict our consideration to the scattering of carriers only on acoustic phonons. Kinetic coefficients were calculated in the one-band approximation by the formulas presented in [3]:

for the differential thermoelectromotive force

$$\alpha = -\frac{k_0}{e}\left(\frac{F_2(\eta)}{F_1(\eta)} - \eta\right), \tag{4}$$

the specific conductivity

$$\sigma = enu\,, \tag{5}$$

here, the carrier mobility

$$u = \frac{e\tau_0(T)}{m^*}\,\frac{F_1(\eta)}{F_{3/2}(\eta)}\,, \tag{6}$$

the heat-conductivity coefficient:

$$\chi = \chi_{\text{lat}} + \mathrm{L}\sigma T\,, \tag{7}$$

where

$$\mathrm{L} = \left(\frac{k_0}{e}\right)^2\left[\frac{F_3(\eta)}{F_1(\eta)} - \left(\frac{F_2(\eta)}{F_1(\eta)}\right)^2\right], \tag{8}$$

here, $F_i(\eta) = \int_0^\infty \left(-\frac{\partial f_0}{\partial x}\right) x^i dx$ is the Fermi integral [3] and $f_0 = [1 + \exp\,(x - \eta)]^{-1}$ is the equilibrium-distribution function. The effective mass of the carrier-state density was taken to be equal to $0.5m_0$ because it is equal to $(0.3–0.7)m_0$ for the best thermoelectric conductors. The dependences of the mobility of charge carriers, the heat conduction of the lattice, and the scattering of charge carriers on their concentration were not taken into account. Let us represent the lattice component of the heat conduction in the form of a temperature dependence:

$$\chi_{\text{lat}} = 326.0/T\,. \tag{9}$$

In the case of scattering of charge carriers on acoustic phonons, the dependence of the carrier mobility on the effective mass and the temperature has the form [3]

$$u = 141.5 {m^*}^{-5/2} T^{-3/2}\,. \tag{10}$$

The coefficients in the equations for the carrier mobility and the lattice heat conduction were selected such that the thermoelectric quality was $3{\cdot}10^{-3}$ K^{-1}, which corresponds to the best thermoelectric conductors at room temperature.

Since the boundary problem (2), (3) is nonlinear, it was solved by numerical methods (the Fermi integrals were also calculated by numerical methods). Simultaneously, we performed numerical optimization with respect to the current and the concentration of charge carriers. The reduced chemical potential was determined from the expression [3]

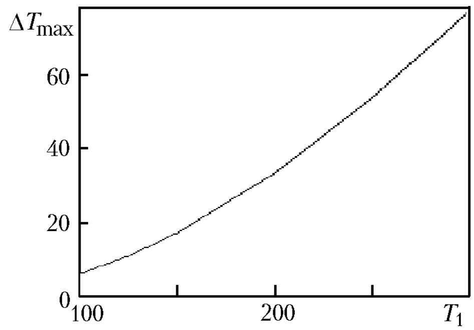


Fig. 1. Dependence of the maximum temperature drop on the temperature of the hot end of a homogeneous arm of a thermocouple.

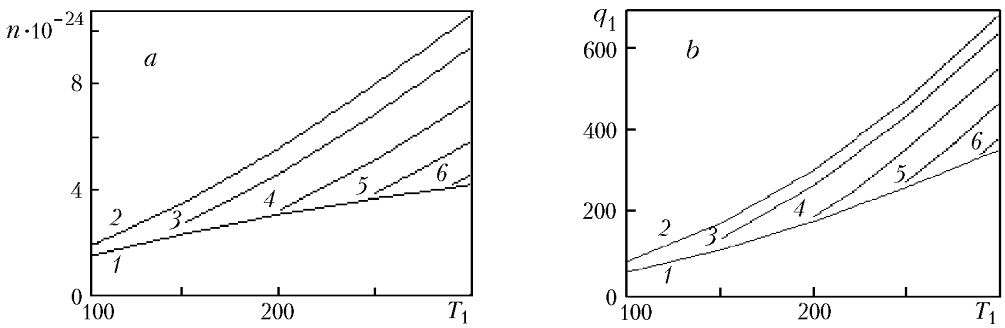


Fig. 2. Dependence of the optimum carrier concentration (a) and the specific heat released at the hot end of an arm of a thermocouple (b) on the hot-end temperature at different temperature drops: ΔT_{max} (1), ΔT = 0 (2), 10 (3), 30 (4), 50 (5), and 70 K (6).

$$n = \frac{8\pi}{3h^3} (2m^* k_0 T)^{3/2} F_{3/2}(\eta) . \tag{11}$$

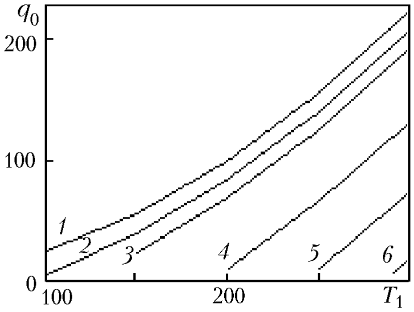
It was established that it varies from –4 to 2.5.

At the hot end of the arm of a thermocouple, the following heat-balance equation is fulfilled:

$$q_1 = \alpha y T \big|_{x=1} - \chi \left. \frac{dT}{dx} \right|_{x=1} . \tag{12}$$

The results of numerically solving the boundary problem are presented graphically. Figure 1 shows the dependence of the temperature drop on the temperature of the hot end of the arm of a thermocouple operating in the regime of maximum temperature drop. It is seen from the graph that, in the case where the temperature dependence of the lattice heat conduction is defined by (9), the thermoelectric conductor is efficient at temperatures that are not lower than room temperature. Simultaneously with numerical solution, we performed numerical optimization of the temperature drop with respect to the concentration of charge carriers. Optimum values of the carrier concentration in the regime of maximum temperature drop are presented in Fig. 2a (curve 1). The dependence of the relative heat (12) released at the hot end of the not-loaded arm on the temperature of this end is presented in Fig. 2b (curve 1), and the dependence of the specific refrigerating capacity of the arm on the temperature of its hot end is presented in Fig. 3. Figure 2 also presents curves of the carrier concentration and the specific heat released at the hot end of the loaded arm at different temperature drops. It is seen that to each regime of operation and each load corresponds its own optimum concentration of charge carriers; this concentration can be determined only by the method proposed.

Since the kinetic coefficients of actual thermoelectric conductors depend on the temperature, only an inhomogeneous arm of a thermocouple can be optimized in the range of operating temperature drops. The use of arms inho-



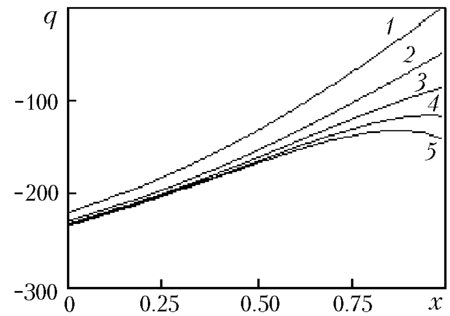


Fig. 3. Dependence of the specific refrigerating capacity of a thermocouple on the temperature of the hot end of its arm at different temperature drops: ΔT = 0 (1), 5 (2), 10 (3), 30 (4), 50 (5), and 70 K (6).

Fig. 4. Distribution of the specific heat flow along the length of an inhomogeneous arm of a thermocouple at different ratios between the carrier concentrations at the cold and hot ends of the arm: n_0/n_1 = 1 (1), 2 (2), 3 (3), 4 (4), and 5 (5).

mogeneous along their length in thermocouples is one way of increasing their thermoelectric efficiency [4]. It was established that the thermoelectric efficiency of a thermocouple increases when the specific conductivity increases and the thermoelectromotive force decreases in the direction from the hot to the cold end of its arm. This conclusion was drawn on the basis of investigation of thermocouples with properties changing gradually along their length; such a thermocouple was considered as a limiting case of a combined thermocouple [4]. It was found that the electrical-conductivity distribution along the arm of this thermocouple is linear.

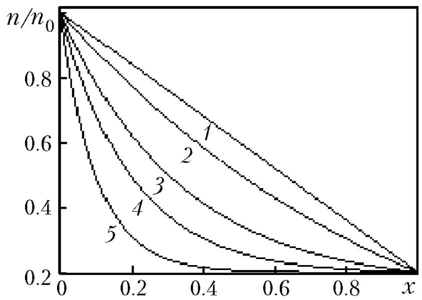
In [5], the thermoelectric efficiency of an arm of a thermocouple was calculated on the basis of solution of the boundary problem. The variational problem formulated by Ivanova and Rivkin [5] was solved using the Pontryagin maximum principle, which necessitated its linearization. It was assumed that the thermoelectromotive force, heat conduction, and electrical conduction, determined on the basis of classical statistics, depend weakly on the temperature. The solution of this problem also has shown that a linear distribution of the charge-carrier concentration along an arm of a thermocouple is optimum.

In [6, 7], this problem was formulated somewhat differently and solved with allowance for the temperature dependence of the kinematic coefficients on the assumption that the carrier-concentration distribution is linear. The regimes of maximum temperature drop and maximum refrigerating capacity were considered. As a result, it has been shown that a linear distribution of the carrier concentration in an arm of a thermocouple is favorable for increasing the temperature drop in it and its refrigerating capacity. A weakness of these works is the use of classical statistics of charge carriers. Since the charge carriers in thermoelectric conductors are somewhat degenerate, we will solve the problem formulated in [7] with the use of the quantum statistics of carriers. The temperature field of an adiabatically isolated, inhomogeneous, one-dimensional arm of a thermocouple operating in a stationary regime is defined, with allowance for the Thomson effect and the distributed Peltier effect, by the stationary heat-conduction equation

$$\frac{d}{dx}\left(\chi \frac{dT}{dx}\right)+\frac{y^2}{\sigma}-yT\left(\frac{d\alpha}{dT}\frac{dT}{dx}+\frac{d\alpha}{dx}\right)=0 \tag{13}$$

with the boundary conditions of (3), where the coefficients α, σ, and χ are calculated by formulas (4), (5), and (7), respectively. The numerical solution of the boundary problem (13), (3) was optimized with respect to the current. Since the nonlinear problem cannot be optimized with the use of the Pontryagin principle and, consequently, an optimum distribution of the carrier concentration cannot be determined, we will consider different concentration distributions along the length of an arm of a thermocouple. Initially, we will analyze a linear distribution of the carrier concentration, which was considered as optimum in [4, 5]:

$$n = n_0\,(1 - gx)\,, \tag{14}$$



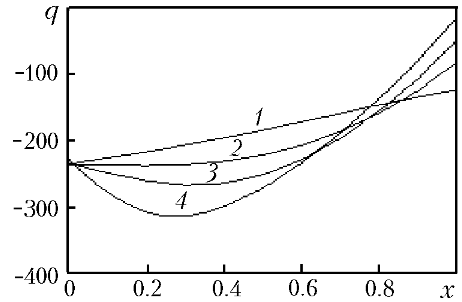


Fig. 5. Distribution of the relative concentration of charge carriers along an arm of a thermocouple at $n_0/n_1 = 5$: linear distribution (curve 1) and exponential distribution with an exponent $a = 1$ (2), 3 (3), 5 (4), and 10 (5).

Fig. 6. Distribution of the specific heat flow along an arm of a thermocouple at a ratio between the carrier concentrations at the cold and hot ends of the arm of $n_0/n_1 = 5$ for different exponents: $a = 1$ (1), 3 (2), 5 (3), and 10 (4).

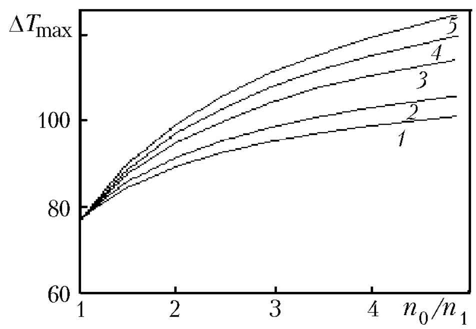


Fig. 7. Dependence of the maximum temperature drop at the cold and hot ends of an arm of a thermocouple on the ratio between the carrier concentrations at these ends n_0/n_1 for $T_1 = 300$ K at different distributions of charge carriers along the arm: linear distribution (curve 1) and exponential distribution with $a = 1$ (2), 3 (3), 5 (4), and 10 (5).

where $g = 1 - 1/k$ ($k = n_0/n_1$ is the ratio between the carrier concentrations at the cold and hot ends of the arm); in this case, $1 \le k \le 5$.

For comparison purposes, it was assumed that the concentration of charge carriers at the cold end of an inhomogeneous arm is equal to that of a homogeneous one. The temperature of the hot end of the arm was constant (300 K). Figure 4 shows the distribution of a specific heat flow along an arm (the sign points to the direction of the heat flow). As follows from the figure, a linear inhomogeneity of an arm leads to a redistribution of the specific heat flow as compared to that in the homogeneous arm (curve 1). It is seen that a temperature maximum is attained at the hot end of the homogeneous arm (curve 1) and, in the inhomogeneous arm, a heat flow increases in the direction from the hot to the cold end. Thus, heat flows are redistributed mainly near the hot end of an arm, and the flow in the neighborhood of the cold end remains practically unchanged. This points to the fact that a linear distribution of charge carriers is insufficiency appropriate. To improve the situation, it is necessary to displace the region of heat absorption in the distributed Peltier effect to the cold end of an arm, for which purpose the distribution of the carrier concentration should be changed by displacement of the region of rapid change in the carrier concentration in the same direction. This change can be attained by increasing the coefficient a in the exponent of the expression

$$n = n_0 (b \exp(-ax) + c), \tag{15}$$

where n_0 is the concentration of charge carriers at the cold end of an arm, $b = (k-1)/[k(1 - \exp(-a))]$, and $c = (1 - k \exp(-a))/[k(1 - \exp(-a))]$.

The relative-carrier-concentration distributions considered in the present work are presented in Fig. 5. The distribution of the specific heat flow along an arm of a thermocouple is shown in Fig. 6. The existence of a carrier-concentration gradient is favorable for decreasing the temperature of the cold end of an arm because of the larger compensation of the Joule heat in this region. However, the heat-flow redistribution caused by a further increase in the difference between the carrier concentrations is no longer favorable for decreasing temperature because an increase in the heat flow happens not at the cold end of the arm. It seems likely that, in order for an optimum concentration distribution to be realized, a large part of the distributed Peltier effect should be transformed into the usual Peltier effect. Figure 7 presents the dependence of the temperature drop on the concentration drop at different concentration distributions along an arm of a thermocouple.

Thus, it has been shown that the concentration of charge carriers in both a homogeneous arm of a thermocouple and an inhomogeneous one should be optimized on the basis of solution of the boundary problem on stationary heat conduction, a linear distribution of the carrier concentration along an arm of a thermocouple is not optimum because it increases the heat flow propagating from the hot end of the arm, and the use of arms with an exponential distribution of the carrier concentration in thermocouples substantially increases their efficiency as compared with thermocouples with arms with a linear distribution of the carrier concentration.

NOTATION

a, b, c, dimensionless coefficients characterizing the concentration distribution; e, elementary charge, C; $F_i(\eta)$, one-parameter Fermi integrals; g, proportionality coefficient; h, Planck constant, J·sec; J, strength of the current flowing in an arm of a thermocouple, A; k, ratio between the concentrations at the cold and hot ends of an arm of a thermocouple; k_0, Boltzmann constant, $J \cdot K^{-1}$; L, Lorentz number, $V^2 \cdot K^{-2}$; l, length of an arm of a thermocouple, m; m_0, free-electron mass, kg; m^*, effective carrier mass, kg; n, concentration of charge carriers, m^{-3}; n_0 and n_1, concentration of charge carriers at the cold and hot ends of an arm of a thermocouple, m^{-3}; Q_0, refrigerating capacity of an arm of a thermocouple, W; Q_1, heat released at the hot end of an arm of a thermocouple, W; $q_0 = Q_0 l/S$, specific refrigerating capacity, $W \cdot m^{-1}$; $q_1 = Q_1 l/S$, specific heat released at the hot end of an arm of a thermocouple, $W \cdot m^{-1}$; S, area of the cross section of an arm of a thermocouple, m^2; T, temperature of an arm of a thermocouple as a function of a coordinate, K; T_1, temperature of the hot end of an arm of a thermocouple, K; u, mobility of charge carriers, $m^2 \cdot V^{-1} \cdot sec^{-1}$; x, dimensionless coordinate, $0 \le x \le 1$; $y = Jl/S$, specific current, $A \cdot m^{-1}$; Z, parameter of thermoelectric efficiency, K^{-1}; α, differential thermoelectromotive force, $V \cdot K^{-1}$; η, reduced chemical potential; σ, specific electrical conduction, $\Omega^{-1} \cdot m^{-1}$; $\tau_0(T)$, relaxation time, sec; χ, specific heat conduction, $W \cdot m \cdot K^{-1}$; χ_{lat}, specific heat conduction of the crystal lattice, $W \cdot m \cdot K^{-1}$. Subscripts: lat, lattice; i, exponent; max, maximum.

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