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Thermopower and resistivity due to dislocations in monovalent metals

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Abstract

Using the partial-wave method, the residual electrical resistivity and the additional and characteristic thermopowers of dislocations for noble and alkaline metals are calculated. Just the scattering of electrons by the dislocation core is considered. The existence of resonance electron states near the Fermi energy within the thermal scatter $k_B T$ is supposed. The lattice dilatation $\Delta V = b_B^2$ (b_B is the steady Burgers vector) is taken into account. Various forms of rectangular potential simulating the dislocation core are investigated. It is shown that unlike the dislocation resistivity, the thermoelectric characteristic of dislocations shows high sensitivity to change of the width of the resonance level and its localization relative to the Fermi energy. A model dislocation potential is suggested; with it, a rather good agreement with available experimental data is obtained.

1. Introduction

It is known that thermopower is very sensitive to any slight changes in the structure and composition of a metal, especially when they cause disturbances of the electronic energy structure near the Fermi surface. The thermopower is closely connected with the electrical resistivity. However, despite significant success in the theoretical explanation of the dislocation residual resistivity [1–6], calculations of additional thermopower due to dislocations are far less common. Except for our early work [7], in which we explained the sign and order of the value of the dislocation contribution to the thermopower for copper, as far as we know, there are no other results in the literature. The fact is that the calculated value of the additional thermopower due to defects depends not only on the value of the scattering cross section, but also on the character of its dependence on the energy near the Fermi surface. For this reason, models of defects used rather successfully for calculation of the residual electrical resistivity appear often to be unsuitable for calculation of the additional thermopower.

The debate in the literature on the disturbances of the crystal lattice caused by dislocations has continued for more than 40 years. It can now be confidently stated that there are two basic mechanisms responsible for the scattering of conduction electrons by dislocations: the first is connected with the long-range elastic strain fields and the second with the short-range

inelastic distortion of the lattice in the dislocation core [8, 9]. The investigations performed during the last few years have shown that a dislocation's elastic strain field causes the small-angle scattering of electrons, whereas the dislocation core causes the large-angle scattering [10, 11]. The former exhibits strong deviation from Matthiessen's rule, i.e. a dependence of the dislocation resistivity per unit dislocation density $\Delta\rho_d/N_d$ on the dislocation density N_d and temperature T . However, the large-angle scattering by the dislocation core is independent of N_d and T at least in a first approximation. The earliest attempts to calculate the residual resistivity of dislocations were connected with the estimation of the influence of the elastic strain fields using linear elasticity theory [12], as well as a second-order elasticity treatment [13, 14]. However, they all resulted in values of $\Delta\rho_d/N_d$ that were too small—almost two orders of magnitude lower than the experimental data. A review of this work is given, for example, in [3] (part 4.1).

Even within linear elasticity theory there is a change of the crystal volume, caused by the dislocation strain field, ΔV_{st} , which is not equal to zero. The total change of the volume due to dislocations ΔV consists of the elastic change of the volume, excluding the area of the core (ΔV_{st}), and the inelastic volume change in the dislocation core (ΔV_{cor}), and $\Delta V \approx b_B^2$ where b_B is Burgers' vector [15–17].

Harrison was the first to consider the inelastic dilatation in the dislocation core for copper, applying the Born approximation [18]. Simulating the dislocation core by a chain of vacancies, he increased the calculated value of $\Delta\rho_d/N_d$ by an order of magnitude. Later, using the partial-wave method with the same dislocation model [2], it became possible to obtain agreement with experiment as regards order of magnitude. However, the attempts to explain the thermoelectric properties of plastically deformed metals within the framework of these representations have failed. It was not possible to explain even the sign of the observed thermoelectric effect [7].

The subsequent progress is connected with the consideration of the dislocation resonance electronic states, localized close to the Fermi surface [3–5]. Their existence for linear defects was predicted by Brown [19]. Later experimental confirmation was obtained by measuring the temperature dependence of the dislocation resistivity for a number of metals (Cu, Al, Mo, W, Zn, Ag, K) [20–23]. To explain the temperature dependence, the presence of additional electron levels on dislocations a few meV above the Fermi level has been assumed [20].

Brown suggested a dislocation resonance model based on a δ -function potential giving electron resonance states at the Fermi surface, and obtained in a calculation of $\Delta\rho_d/N_d$ quite a good agreement with experiment for a large number of non-transition metals [3]. However, this model had a number of drawbacks, such as the fact that the results are independent of the value of the Burgers vector and the orientation of the dislocations relative to the electrical current, and also the neglect of the lattice dilatation in the dislocation core.

Our dislocation model is devoid of these shortcomings. The model proved quite successful in the calculation of $\Delta\rho_d/N_d$ for a wide range of monovalent, polyvalent, and transition metals [5]. In the present work we investigate this model and show that it can be applied successfully for the calculation not only of the dislocation resistivity but also the thermoelectric characteristics of dislocations. Only monovalent metals (i.e. noble and alkaline) will be considered, as their Fermi surfaces are simpler and better measured, and consequently can be taken into account in the calculations of the thermopower more precisely.

2. Approaches to and method of calculation

We believe that the dislocation core gives rise to the major contribution to the electron scattering and change of the electron-transfer properties. The scattering due to the long-range elastic strain fields surrounding the dislocation can be neglected, because their influence is several tens of

times weaker both for separate dislocations and for dislocation arrays [24]. The influence of dislocations on the resistivity and diffusion thermopower is considered assuming the validity of Matthiessen's rule.

The scattering cross section of the dislocation is calculated by the partial-wave method (PWM). It should be noted that the PWM is an exact scattering theory method, and it allows one to choose one parameter of the scattering potential self-consistently, taking into account the screening effects [8]. As a result, the calculated cross section is almost independent of the form of the scattering potential, and the more complicated Coulomb potentials can be replaced by simpler square ones without loss of precision.

First, as a scattering potential, we considered an axially symmetrical potential used earlier for calculation of the dislocation resistivity in [5]:

$$V(r) = \begin{cases} V_1 & r < R_1 \\ V_0 & R_1 \leq r \leq R_2 \\ 0 & r > R_2. \end{cases} \quad (1)$$

This potential is one of the simplest that permits one to take into account the main features of the perturbation of the crystal lattice in the dislocation core—that is, the dilatation of the crystal lattice, and the existence of resonance quasi-stationary electron states in the area of positive values of energy, in particular near the Fermi energy. Such a form of potential reflects real distortion of the lattice in the dislocation core, namely the existence of a compressing area side by side with the expanding one, which can capture the conduction electrons forming short-lived states. Although the scattering potential for individual dislocations is non-axially symmetrical (especially for an edge dislocation), the average dislocation potential for a polycrystal with a random dislocation distribution may be considered as axially symmetrical.

In view of the fact that the dislocation length is much greater than the width of the dislocation core, the edge effect can be neglected, which allows one to regard just the perpendicular component of the wavevector $k_{\perp} = k \sin \varphi$ as changing during the scattering (here k is the value of the wavevector at the Fermi level and φ is the angle between the dislocation axis and vector \mathbf{k}).

The solution of the Schrödinger equation for potential (1) is given in [5] in detail. The expressions for the phase shifts η_m are given there too; they represent a superposition of potential (α_m) and resonant (β_m) components:

$$\eta_m = \alpha_m + \beta_m \quad (2)$$

where

$$\beta_m = \arctan \frac{\Gamma_m}{2(E_{r,m} - E_{\perp})}.$$

Here, $E_{\perp} = k_{\perp}^2 = k^2 \sin^2 \varphi$, $E_{r,m}$ and Γ_m are the position and width of the m th resonance level. The width of the level Γ_m determines the lifetime of this electron state, $\tau_m \sim \hbar / \Gamma_m$.

Now we shall stop briefly to consider the choice of potential parameters. The external radius R_2 is determined from the value of the lattice dilatation in the dislocation core ΔV . According to [15], $\Delta V = b_B^2$ per unit of dislocation length; thus $R_2 = b_B / \sqrt{\pi}$. As the vector \mathbf{b}_B , we take the steady Burgers vector of the full dislocation; thus for FCC metals, it is $(1/2)\langle 110 \rangle$ and has the value $a_0 / \sqrt{2}$ (a_0 is the lattice parameter). For such a choice, the value of R_2 is close to the atomic radius for cubic structures.

The height of the potential barrier V_0 is determined self-consistently from the screening condition (the Friedel sum rule), which for linear defects has the form [13]

$$\frac{k}{\pi^2} \int_0^{\pi} \sum_{m=-\infty}^{\infty} \eta_m(\varphi) \sin \varphi \, d\varphi = \xi \quad (3)$$

where ξ is the line density of charge along the dislocation axis, expressed in terms of the quantity of electron charge as $\xi = n_s \Delta V / \Omega_a$, where Ω_a is the atomic volume and n_s is the number of carriers per atom (for monovalent metals, $n_s = 1$). The left-hand side of (3) represents the number of additional electronic states created by the charged linear defect per unit dislocation length.

The localization of resonance states depends on the depth of the potential well V_1 . The criterion for choice of the value of V_1 is based on the assumption that the dislocation resonance levels are close to the Fermi energy—within the thermal scatter $k_B T$:

$$|E_r - E_F| \leq k_B T \quad (4)$$

because electrons with such energy take part in the electron-transfer process and in that case their interaction with the resonance states will be the most intense. Only the zero level $E_{r,0}$ satisfies condition (4); the levels $E_{r,m}$ for $m \geq 1$ were too far from the Fermi energy and were not taken into account (from here on, $E_{r,0} \equiv E_r$).

The last parameter of the potential is the internal radius R_1 ; it is a free parameter in the analysis. Change of this parameter varies the width and consequently the lifetime of the resonance state. We assumed in [5] that $R_1 = R_2/2$, and it was noted there that the variation of R_1 does not significantly influence the scattering cross section if the height of the potential V_0 is chosen self-consistently. In the present work will investigate, in more detail, how the variation of the parameter R_1 affects the results on the calculated electrical resistivity and thermopower due to dislocations.

The transport scattering cross section averaged over all possible directions of the wavevector relative to the dislocation axis can be presented as a superposition of the resonance (Q_R), potential (Q_P), and interference (Q_I) components [25]:

$$\begin{aligned} Q &= \frac{1}{2k} \int_0^\pi \left(\frac{\Gamma^2}{(E_\perp - E_r)^2 + \Gamma^2/4} - \frac{2[\Gamma^2 \sin \delta_0 - \Gamma(E_\perp - E_r) \sin(2\delta_0)]}{(E_\perp - E_r)^2 + \Gamma^2/4} \right. \\ &\quad \left. + 4 \sum_{m=0}^{\infty} \sin^2 \delta_m \right) d\varphi \\ &= Q_R + Q_I + Q_P = \frac{2}{k} \int_0^\pi \sum_{m=0}^{\infty} \sin^2(\eta_m - \eta_{m+1}) d\varphi \end{aligned} \quad (5)$$

where $\delta_m = \alpha_m - \alpha_{m+1}$.

The potential and resonant components are always positive. The interference component Q_I is negative for the negatively charged defect. Thus, the interference of the potential and resonant scattering results in the general scattering cross section Q being less than the sum of the potential and resonance ones. Moreover, if the line charge density of the defect ξ is fairly large, the value of Q can even be less than the potential component Q_P . The dependence of the general cross section Q and its components Q_P , Q_R , and Q_I on the electron energy E for copper are presented in figure 1 (corresponding curves: 2, 1, 5, and 6). Here $E_r = E_F$ is assumed; this energy is shown by a vertical line. The maximum of the resonance peak is displaced considerably to the right relatively to the resonance energy E_r . The main cause of this displacement is that here a random orientation of dislocations is considered and the scattering cross section is averaged over the angle φ . When all of the dislocations are perpendicular to the current direction (that is, $k_\perp = k$), the maximum of the resonant peak coincides with the resonance energy (curve 4). It is obvious that in this case the maximum value of the scattering cross section is higher.

The change of the electrical resistivity due to dislocations per unit of their density, within

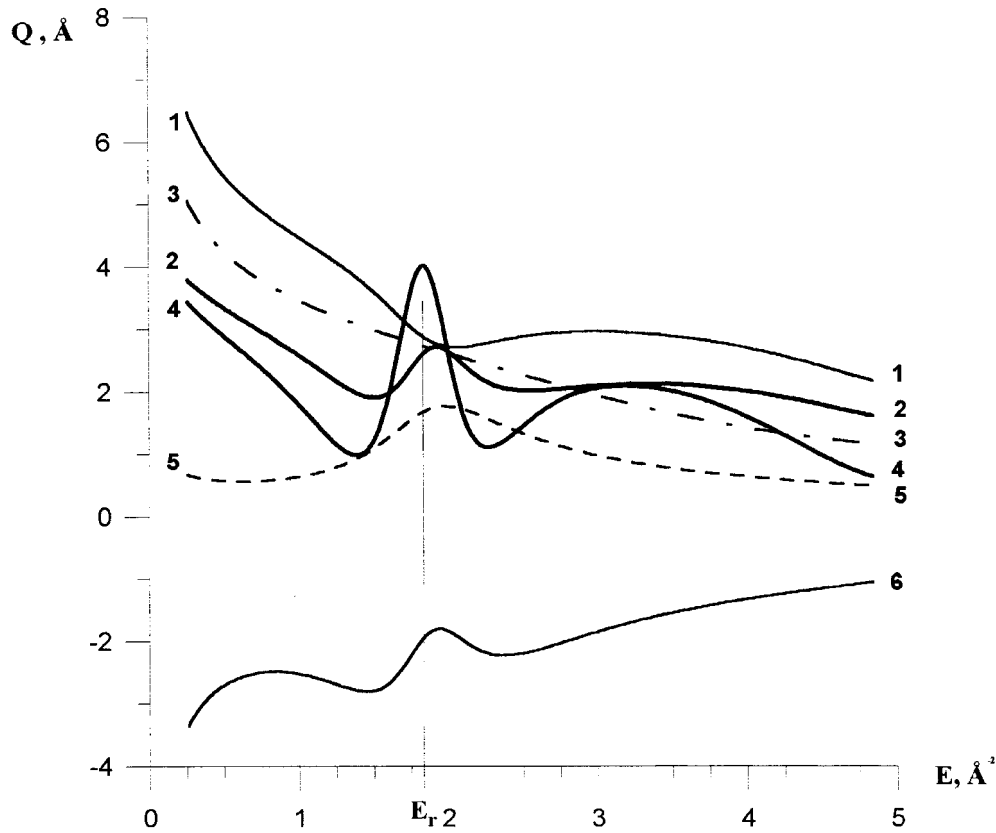


Figure 1. The dependence of the scattering cross section Q and its resonance (Q_R), potential (Q_P), and interference (Q_I) components on the electron energy E for copper: 1: Q_P ; 2: Q ; 5: Q_R ; 6: Q_I ; 4: $Q(E)$ for normal incidence of electrons on the dislocation axis ($k_{\perp} = k$); 3: $Q(E)$ for the cylindrical potential barrier ($n = 0$).

the relaxation-time approximation, is defined by

$$\frac{\Delta\rho_d}{N_d} = \frac{\hbar k \Omega_a Q}{n_s e^2}. \quad (6)$$

The change of the absolute thermopower due to a unit of dislocation density (additional thermopower) is estimated from the expression [26]

$$\frac{\Delta S_d}{N_d} = S_0 \frac{\Delta\rho_d}{\rho N_d} \left(\frac{\Delta x}{x} - 1 \right) \quad (7)$$

where $\rho = \rho_0 + \Delta\rho_d$, and

$$x = - \left(\frac{\partial \ln \rho_0}{\partial \ln E} \right)_{E=E_F}$$

$$\Delta x = - \left(\frac{\partial \ln \Delta\rho_d}{\partial \ln E} \right)_{E=E_F} = - \frac{k}{2Q} \left(\frac{\partial Q}{\partial k'} \right)_{k'=k} + \left(\frac{\partial \ln F}{\partial \ln E} \right)_{E=E_F} = \Delta x_Q + \Delta x_F.$$

Here S_0 and ρ_0 are the absolute thermopower and electrical resistivity of annealed metal at temperature T ; k_B is the Boltzmann constant; e is the electron charge; F is the area of the Fermi surface. These expressions are correct for temperatures $T \ll T_D$ and $T \gg T_D$ (here T_D

is the Debye temperature), where it is possible to neglect the phonon-drag effect and inelastic scattering of electrons by phonons and defects [26].

The characteristic thermopower of the dislocations is

$$S_d = \frac{\pi^2 k_B^2 T}{3|e|} \left(\frac{\partial \ln \Delta \rho_d}{\partial E} \right)_{E=E_F} = -\frac{\pi^2 k_B^2 T}{3|e|E_F} \Delta x. \quad (8)$$

Thus, to calculate the thermoelectric characteristics of dislocations it is necessary to know the values of the parameters Δx_F and Δx_Q . The theoretical estimates of Δx_F differ substantially between various studies and remain far from the experimental values; in the present work, as the value of Δx_F , the magnitude obtained from the thermoelectric size-effect measurements is taken [27]. Among the available experimental data, preference was given to those which were measured for foils. The results obtained on the thin films show a wide scatter of values, because of the uncontrolled impurity contents and the high concentration of defects, which sometimes have a great dependence on the film thickness (the false size effect). In view of the absence of reliable experimental data for alkaline metals, as the value of Δx_F the free-electron-model value is taken: $\Delta x_F = 1$, in view of the closeness of their Fermi surfaces to the free-electron sphere [28].

The derivative $(\partial Q/\partial k')_{k'=k}$ needed for calculation of Δx_Q was approximated by the average value of the ratio obtained for a change of k by about $\pm 0.001 \text{ \AA}$. Decrease of the interval of differentiation by an order of magnitude did not change the average value up to the third digit. Summing over m was carried out up to $m = 10$; the screening condition (3) was fulfilled within an accuracy of 10^{-4} .

3. Results and discussion

In the work described, all parameters of the potential (except R_1) are determined quite unambiguously. Therefore it was necessary to estimate first of all how the change of radius R_1 influences the results for the electrical characteristics of dislocations. The variation of R_1 was defined through the coefficient n , showing what part of R_1 arises from R_2 ; that is, $R_1 = nR_2$. The coefficient n was changed from 0 to 0.9. The results of this analysis for copper are given in table 1. These are: the variation of the dislocation electrical resistivity $\Delta \rho_d/N_d$; thermoelectric parameters Δx_Q , Δx ; the potential parameters V_1 , V_0 ; and the width of the resonance level Γ for $E_r = E_F$ ($\Delta x_F = -1.20$ [27]).

At $n = 0$ we have a simple cylindrical potential barrier of height V_0 with radius R_2 ; quasi-stationary states are absent for such a potential. Such a model of dislocations reflects only the fact of lattice dilatation in the area of the dislocation core which creates a negative surplus charge in the lattice. It is obvious that in this case the parameter Δx_Q takes on a classical value equal to 0.5. The dependence $Q(E)$ for $n = 0$ is shown by the chain line in figure 1 (curve 3).

It is obvious that the variation of n from 0 to 0.9 results in a change of the dislocation residual resistance, from 1.95 to $1.76 \times 10^{-13} \mu\Omega \text{ cm}^3$; this is by about 10%. The measured values of the dislocation resistivity $(\Delta \rho_d/N_d)^{exp}$ for copper are within the interval $(1.3-2.3) \times 10^{-13} \mu\Omega \text{ cm}^3$ [10]; more rigorous analysis gives $(1.6 \pm 0.2) \times 10^{-13} \mu\Omega \text{ cm}^3$ [3]. Therefore, the calculated value of $\Delta \rho_d/N_d$ agrees quite well with the measured one for any R_1 . However, a different situation arises for the calculated thermoelectric characteristics of the dislocations. As is seen from table 1, the value of Δx_Q has more than doubled in magnitude over the same range of variation of R_1 , and has even changed in sign; the value of Δx , proportional to S_d , has altered substantially too. This means that there is an obvious ambiguity in the choice of radius R_1 in the calculation of the dislocation thermoelectric characteristics. Thus, potential

Table 1. The dependence of the scattering parameters and electrical characteristics of the dislocations on the value of the internal radius R_1 of potential (1) for copper.

n	V_0 (eV)	V_1 (eV)	Γ (eV)	$\Delta\rho_d/N_d$ ($10^{-19} \Omega \text{ cm}^3$)	Δx_Q	Δx
0	6.50	—	0	1.79	0.50	-0.70
0.1	17.39	125.05	1.14	1.95	-0.73	-1.93
0.3	18.83	23.68	1.30	1.91	-0.84	-2.04
0.5	21.66	10.41	1.64	1.90	-0.95	-2.15
0.7	29.55	3.62	1.87	1.84	-1.14	-2.34
0.9	68.63	0.53	2.90	1.76	-1.35	-2.55

(1), which is quite suitable for calculation of the dislocation resistivity, appears to be unsuitable for calculation of the dislocation thermopower.

To eliminate the uncertainty in the choice of the parameter R_1 , the scattering potential of the dislocation core was simplified and replaced by the potential

$$V(r) = \begin{cases} 0 & r < R_1 \\ V_0 & R_1 \leq r \leq R_2 \\ 0 & r > R_2. \end{cases} \quad (9)$$

This is the same potential as we used earlier for calculation of the dislocation contribution to the thermopower of copper [7]. This potential is a particular case of potential (1), but it does not have any ambiguous parameter affecting the form of the potential, which is important for the thermopower calculation. Now the internal radius R_1 is determined from condition (4).

The results of the calculation with the potential (9) for temperature $T = 273 \text{ K}$ are listed in table 2. There are also the parameters used for the material: a_0 , S_0 , and ρ_0 . The values of the parameter Δx_F for Cu, Ag, and Au are respectively -1.20 , -1.91 , and -1.05 [27]. For comparison, the available experimental data on the residual dislocation resistivity $(\Delta\rho_d/N_d)^{exp}$ are presented. It is obvious that the agreement with our results is quite good, especially for noble metals, for which the experimental data are more reliable.

The comparison of the results obtained for the thermopower with experiment is rather laborious, as the quantitative characteristics of the dislocation contribution to the thermopower are very poor and are presented only for noble metals in references [29, 30]. Polak reported measurements of the change of electrical resistivity $\Delta\rho$ and thermopower ΔS due to defects introduced by plastic deformation (mainly dislocations) in gold [29]. It was found that the ratio $\Delta S/\Delta\rho = 0.76 \text{ V K}^{-1} \Omega^{-1} \text{ cm}^{-1}$, and the thermoelectric parameter $\Delta x = -2.5$. The results presented here for gold are respectively $\Delta S_d/\Delta\rho_d = 0.61 \text{ V K}^{-1} \Omega^{-1} \text{ cm}^{-1}$ and $\Delta x = -2.48$. The characteristic thermopower of dislocations measured at room temperature for noble metals by Likhvich is close to $2 \mu\text{V K}^{-1}$ [30]. The values of S_d calculated here for these metals at the same temperature are in the range from 2.6 to $4.3 \mu\text{V K}^{-1}$. Thus, one may state that there is a quite satisfactory agreement of the calculated thermoelectric characteristics of the dislocations with the available experimental data.

As follows from expression (7), the change of the thermopower per unit of dislocation density $\Delta S_d/N_d$ and also the ratio $\Delta S_d/\Delta\rho_d$ should not depend substantially on the temperature in the range of quasi-elastic scattering of electrons on phonons and defects ($T \ll T_D$ and $T \geq T_D$), where S_0 and ρ_0 show practically linear dependences on the temperature.

From comparison of the results for copper obtained with the different potentials (1) and (9), which are presented in tables 1 and 2, one may conclude that: firstly, the change of the level width slightly influences the value of the dislocation resistivity, but substantially alters

Table 2. Parameters of the calculation and the electrical characteristics of dislocations in monovalent metals for $E_r = E_F$ ($T = 273$ K).

Metal	a_0 (Å) [31]	ρ_0 ($\mu\Omega$ cm) [8]	S_0 (μ V K ⁻¹) [27]	Γ (eV)	Δx_Q
Cu	3.615	1.55	1.71	3.10	-1.43
Ag	4.086	1.50	1.38	2.44	-1.43
Au†	4.078	2.04	1.74	2.44 2.48	-1.43 -1.54
Li	3.509	8.50	10.60	2.19	-1.89
K	5.211	6.30	-12.80	1.00	-1.87
Cs	6.062	19.00	-0.90	0.74	-1.87

Metal	$\Delta\rho_d/N_d$ (10^{-19} Ω cm ³)	$\Delta\rho_d/N_d$ (10^{-19} Ω cm ³) (experiment)	S_d (μ V K ⁻¹)	$\Delta S_d/N_d$ (10^{-19} V cm ² K ⁻¹)	$\Delta S_d/\Delta\rho_d$ (V K ⁻¹ Ω^{-1} cm ⁻¹)
Cu	1.73	1.6 ± 0.2 [3] 1.7 [32]	2.49	0.86	0.50
Ag	2.49	1.9 [32] 3.1 [33]	4.03	4.40	1.77
Au†	2.48 2.47	2.6 [32]	2.98 3.12	1.51 1.66	0.61 0.67
Li	2.93		1.26	-3.22	-1.10
K	9.60	4 [32]	2.72	23.65	2.46
Cs	15.12		3.69	3.65	0.24

†The second line for gold presents results at $E_r = E_F + k_B T$.

the thermopower; secondly, different forms of potentials give approximately identical values of $\Delta\rho_d/N_d$ and S_d , if they (other conditions being equal) result in close widths of the resonance levels (Γ). One may note, for comparison, that different scattering potentials give rather close values of the scattering cross section and values of $\Delta\rho_d/N_d$ if they satisfy the same screening condition (the Friedel sum rule); that is, the value of the residual resistivity carries information mainly about the value of the surplus charge of the defect.

To find out how sensitive the results are to the position of the resonance level with respect to the Fermi energy, the results for copper were recalculated for the resonance energy $E_r = E_F + \Delta$, where $\Delta = \pm nk_B T$ (here $k_B T = 0.023$ eV). The results are presented in table 3.

It is obvious that the shift of E_r by an amount of the order of magnitude of $k_B T$ (here, up to $12 k_B T$) leads to a small change of the dislocation resistivity whereas the additional thermopower varies rather substantially. So the value of $\Delta\rho_d/N_d$ for copper changes by a few per cent (no more than 12%) and remains practically within the error of the measurements, whereas the value varies by several times and even reverses in sign. This indicates that the thermoelectric characteristics of the defects can give quantitative information about the localization of electronic states on the defects relative to the Fermi energy.

4. Conclusions

Thus, the dislocation model, proposed by us earlier, explains rather well not only the contribution of dislocations to the electrical resistivity for a wide range of metals [5], but

Table 3. Influence of the shift E_r relative to E_F on the dislocation resistivity and thermopower in copper ($E_r = E_F \pm nk_B T$) for $T = 273$ K.

Δ ($k_B T$)	E_r (eV)	Γ (eV)	Δx_Q	$\Delta\rho_d/N_d$ ($10^{-19} \Omega \text{ cm}^3$)	$\Delta S_d/N_d$ ($10^{-19} \text{ V cm}^2 \text{ K}^{-1}$)
0	7.036	3.10	-1.43	1.73	0.86
1	7.059	3.15	-1.51	1.72	0.94
-1	7.013	3.49	-1.38	1.65	0.77
4	7.128	3.22	-1.80	1.67	1.21
-4	6.944	3.85	-1.18	1.58	0.55
8	7.220	3.34	-2.11	1.60	1.46
-8	6.852	4.12	-0.91	1.55	0.28
12	7.312	3.45	-2.37	1.52	1.63
-12	6.760	4.38	-0.58	1.53	-0.03

also the available experimental data on the dislocation contribution to the thermopower for noble metals (the results for $\Delta S_d/N_d$ for alkaline metals still require an experimental check).

The basic features of this model are following:

- the dislocation core gives rise to the dominant contribution to the change of the electron-transfer properties caused by dislocations;
- the lattice dilatation in the dislocation core has a value of about b_B^2 which determines the linear surplus charge of the defect and its radius;
- the existence of the compressing area side by side with the expanding one leads to capture of conduction electrons, forming short-lived quasi-stationary states near the Fermi energy ($\pm k_B T$).

However, the model potential used earlier for calculation of $\Delta\rho_d/N_d$ [5] appears to be unsuitable for calculation of $\Delta S_d/N_d$, because it contains an ambiguously determined parameter of the potential form. Changing the parameter results in a change of the resonant level width that hardly influences the results for $\Delta\rho_d/N_d$, but substantially affects the results for $\Delta S_d/N_d$. Another model potential is proposed which appears to work quite well in calculations of the resistivity and thermopower due to dislocations for monovalent metals.

On the basis of the research performed, one may conclude that, unlike the residual resistivity, the additional and characteristic thermopower are very sensitive to the change of width of the resonance level and its localization near the Fermi energy.

Therefore, whereas the residual resistivity of defects carries information mainly about the value of the excess charge of defects in the lattice and does not depend significantly on the form of the scattering potential (if the Friedel sum rule is fulfilled), the thermoelectric characteristics of the defects contain additional information about the quasi-stationary electron states localized on the defects, their energies, and the lifetimes, and depend substantially on the form of the scattering potential.

Thus the thermopower not only is highly sensitive, but also is a highly informative property. The experimental data on the contribution of defects or impurity to the thermopower can give quantitative information about the localization of the electron states close to the Fermi surface. So our results for gold correlate better with experiment at $E_r = E_F + k_B T$ (these results are given in the second line for Au in table 2); this means that the dislocation resonance states in gold are located above the Fermi energy by about $k_B T$. That correlates with the conclusion reached in [20]. One would like to hope that there will be an expansion of experimental research into the thermoelectric properties of defects in the near future; that should provide

new information on the electron states on defects and further develop the electron-transfer theory.

References

- [1] Brown R A 1977 *J. Phys. F: Met. Phys.* **7** 1283–95
- [2] Likhvich A A and Karolik A S 1978 *Fiz. Met. Metalloved.* **45** 863–5 (in Russian)
- [3] Brown R A 1982 *Can. J. Phys.* **60** 766–78
- [4] Föckel H-J 1987 *Phys. Status Solidi b* **139** 59–66
- [5] Karolik A S and Likhvich A A 1994 *J. Phys.: Condens. Matter* **6** 873–86
- [6] Watts B R 1988 *J. Phys. F: Met. Phys.* **18** 1197–209
- [7] Likhvich A A and Karolik A S 1982 *Fiz. Met. Metalloved.* **54** 909–14 (in Russian)
- [8] Blatt F J 1968 *Physics of Electronic Conduction in Solids* (New York: McGraw-Hill)
- [9] Trattner D, Zehetbauer M and Gröger V 1985 *Phys. Rev. B* **1172–3**
- [10] Zehetbauer M 1989 *J. Phys.: Condens. Matter* **1** 2833–41
- [11] Zürcher R *et al* 1995 *J. Phys.: Condens. Matter* **7** 3515–28
- [12] Hunter S C and Nabarro F R N 1953 *Proc. R. Soc. A* **220** 542–61
- [13] Stehle H and Seeger A 1956 *Z. Phys.* **146** 217–68
- [14] Seeger A and Bross H 1960 *Z. Naturf. a* **15** 663–89
- [15] Shmatov V T 1975 *Fiz. Met. Metalloved.* **40** 910–19
- [16] Seeger A and Haasen P 1958 *Phil. Mag.* **3** 470–5
- [17] Seeger A 1958 *Nuovo Cimento* **7** 632–45
- [18] Harrison W A 1958 *J. Phys. Chem. Solids* **5** 44–6
- [19] Brown R A 1967 *Phys. Rev.* **156** 692–700
- [20] Gantmakher V F and Kulesko G I 1975 *J. Phys.: Condens. Matter* **19** 151–60
- [21] Gantmakher V F and Kulesko G I 1975 *Sov. Phys.–JETP* **40** 1158–60
- [22] Endo T and Kino T 1979 *J. Phys. Soc. Japan* **46** 1515–21
- [23] Guban D 1971 *Proc. R. Soc. A* **325** 223
- [24] Sacks R A and Robinson J E 1976 *Phys. Rev. B* **13** 611–20
- [25] Likhvich A A and Karolik A S 1984 *Fiz. Met. Metalloved.* **58** 1076–9 (in Russian)
- [26] Blatt F J, Shroeder P A, Foiles C L and Graig D 1976 *Thermoelectric Power of Metals* (New York: Plenum)
- [27] *Landolt–Börnstein New Series* 1982 Group III, vols 15a, b (Berlin: Springer)
- [28] Ashcroft N W and Mermin N D 1976 *Solid State Physics* (New York: Holt, Rinehart and Winston)
- [29] Polak J 1964 *Czech. J. Phys. B* **14** 176–88
- [30] Likhvich A A 1976 *Vlijanie Defektov na Electrichekieskie Svoistva Metallov* (Minsk: Nauka i Tekhnika) (in Russian)
- [31] Mirkin L I 1961 *Spravochnik po Rentgenostrukturnomu Analizu Policristallov* (Moscow: GI Fiz.-Mat. Literat.) (in Russian)
- [32] Basinski Z S, Dugdale J S and Howie A 1963 *Phil. Mag.* **8** 1989–97
- [33] Kovacs I and Nagy E 1965 *Phys. Status Solidi* **8** 795–803