TEMPERATURE DEPENDENCE OF THE SHAKE-OFF EFFECT FOR CONDUCTIVITY ELECTRONS IN METALS

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We analyzed the emission of the conduction electrons in metals caused by any nuclear decay. The refraction of the electron wave at the crystal surface, as well as its attenuation due to scattering by phonons, are taken into account. It is shown that the energy distribution of ejected shake-off electrons contains a peak at the energy of the order of 1 eV, whose intensity falls down with growing temperature. The dependence of the yield of conduction electrons on the thickness of a radioactive source is studied as well.

1. Introduction

For a long time, the problem of the emission of low-energy electrons from targets, following any nuclear transmutation, attracts a great attention [1–18]. The electrons around the nucleus apprehend its charge alteration as a sudden perturbation of the Coulomb field, which gives rise to their emission from the target. The energy of emitted shake-off electrons equals a few eV. Previously, all theorists have been concentrating on the shake-off effect for electrons initially bound on deep K and L levels of an isolated atom. The emission probability of these electrons is too small as compared with that from experimental data. In particular, the estimations in [3] show that the probability for the emission of a K electron after the beta-decay only is $3/4Z^2$, where Z stands for the atomic number. At the same time, experiments [12] indicate that the average yield of low-energy electrons after the β decay of a single nucleus ^{154}Eu in a thin source is $n_\beta = 0.5$. Such a discrepancy can be easily understood, by applying standard formulas of the sudden perturbation theory [19] which predict a quick decrease of the electron emission probability with increase in their binding energy. Therefore, it can be stated that experimentalists mainly observe the shake-off electrons initially bound on the upper levels. In metals, such levels belong to the conduction band.

In our previous paper [18], the shake-off effect was first analyzed for valent electrons in metal crystals within the simplest model. The electrons were treated as noninteracting particles moving in a rectangular potential well

$$U(\mathbf{r}) = \begin{cases} -U_0, & \text{inside the crystal,} \\ 0, & \text{outside it} \end{cases} \tag{1}$$

with wave vectors $\mathbf{q}$. The depth of the potential well equals

$$U_0 = \varepsilon_{\rm F} + A, \tag{2}$$

where $\varepsilon_{\rm F} = \hbar^2 q_{\rm F}^2/2m$ is the Fermi energy, and A is the work function.

When a nucleus decays at some distance z_s from the surface of the crystal slab, it suddenly perturbs the Coulomb field at this point and gives rise to a spherical outgoing electron wave with the origin at the nucleus. Such spherical wave may be decomposed into the plane waves $e^{i\mathbf{Kr}}$ which are refracted at the surface, bearing the waves $e^{i\mathbf{kr}}$ in vacuum. If the shake-off electron has the energy $E = \hbar^2 k^2/2m$, then the obvious equality holds:

$$E = \epsilon - U_0. \tag{3}$$

Here, $\epsilon = \hbar^2 K^2/2m$ represents the kinetic energy of the electron inside the crystal.

Due to the inelastic scattering of an electron wave by vibrating ions of the crystal, the wave vector $\mathbf{K}$ attributes the imaginary part. As a result, the intensity of the electron beam which passed the distance x in the medium exponentially decreases:

$$I(x) = I(0)e^{-\mu x}. \tag{4}$$

Here, the attenuation coefficient depending mainly on the scattering by phonons is

$$\mu = \sigma_{\rm in}/v_0, \tag{5}$$

where $\sigma_{\rm in}$ is the inelastic scattering cross section of electrons by phonons referred to one atom, and v_0 is the volume of the elementary cell (we assume that it contains one atom).

In this article, we will study the role of the attenuation of a shake-off electron wave in the crystal. For this aim, we calculate the inelastic cross section $\sigma_{\rm in}$ for the scattering of electrons with absorption or emission of phonons which depends significantly on the temperature. Earlier, $\sigma_{\rm in}$ was calculated in the long-wave approximation for low-energy conduction electrons, regarding the crystal as a continuous medium (see, e.g., [20]). But, in our case, the electrons inside the crystal have kinetic energy ϵ of the order of 10 eV and higher, which forces us to give a more refined derivation. Having found formulas for $\sigma_{\rm in}$, we are able then to analyze the effects related to the attenuation of shake-off electrons in the medium.

It is worth to note that a similar picture arises when fast ions flying through microstrip metal detectors provide the emission of a great number of low-energy electrons [21]. Therefore, the investigation of various aspects of low-energy electron emission from metal films become today the most actual.

2. Attenuation of an Electron Wave

In this section, we will calculate the inelastic scattering cross section $\sigma_{\rm in}$ of electrons by phonons in a perfect crystal which enters the attenuation coefficient (5). We recall that we consider the crystal with one atom per unit cell, whose position is defined by the vector

$$\mathbf{R}_{\mathbf{l}} = \mathbf{l} + \mathbf{u}_{\mathbf{l}}, \tag{6}$$

where $\mathbf{l}$ is the lattice vector, and $\mathbf{u}_{\mathbf{l}}$ is a displacement of the ion from its equilibrium position.

The perturbation operator is given by

$$\hat{V}(r) = \sum_{\mathbf{l}} [v_c(|\mathbf{r} - \mathbf{R}_{\mathbf{l}}|) - v_c(|\mathbf{r} - \mathbf{l}|)], \tag{7}$$

where $v_c(r)$ is the Coulomb interaction energy of the electron with an ion,

$$v_c(r) = -\frac{Ze^2}{r} e^{-r/r_0}, \tag{8}$$

depending on the screening length r_0.

The initial state of the system (crystal lattice + electron) is described by the function

$$|a\rangle = |\{\nu_{\boldsymbol{\kappa}j}\}\ \rangle\ e^{i\mathbf{K}\mathbf{r}}, \tag{9}$$

where $\nu_{\boldsymbol{\kappa}j}$ denotes the number of phonons specified by a quasiwave vector $\boldsymbol{\kappa}$, branch number j, and frequency $\omega_j(\boldsymbol{\kappa})$. The final wave function will be

$$|b\rangle = |\{\nu'_{\boldsymbol{\kappa}j}\}\ \rangle\ e^{i\mathbf{K}'\mathbf{r}}. \tag{10}$$

The cross section for the transition from $|a\rangle$ to $|b\rangle$ is given by

$$\sigma_{a\to b} = \frac{2\pi}{\hbar v} |V_{ba}|^2 \delta(E_b - E_a), \tag{11}$$

where $v = \hbar K/M$ is the velocity of incident electrons, and the matrix element in the Born approximation is determined by the expression

$$V_{ba} = \frac{4\pi Z e^2 r_0^2}{1 + Q^2 r_0^2} \sum_{\mathbf{l}} \left\langle \{\nu'_{\boldsymbol{\kappa}j}\} | e^{i\mathbf{Q}(\mathbf{l}+\mathbf{u}_{\mathbf{l}})} | \{\nu_{\boldsymbol{\kappa}j}\} \right\rangle \tag{12}$$

with the scattering vector

$$\mathbf{Q} = \mathbf{K} - \mathbf{K}'. \tag{13}$$

In the single-phonon approximation, the inelastic scattering cross section of electrons by a crystal is given by

$$\sigma_{\rm in}^{(N)} = \frac{2\pi}{\hbar v} \int \frac{d\mathbf{K}'}{(2\pi)^3} \sum_{\boldsymbol{\kappa}j} \left(\frac{4\pi Z e^2 r_0^2}{1 + Q^2 r_0^2} \right)^2 \times$$
$$\times e^{-2W(\mathbf{Q})} \frac{\hbar}{2NM\omega_j(\boldsymbol{\kappa})} |\mathbf{Q}\ \mathbf{e}_j(\boldsymbol{\kappa})|^2 \times$$
$$\times \left[\left| \sum_{\mathbf{l}} e^{i(\mathbf{Q}+\boldsymbol{\kappa})\mathbf{l}} \right|^2 \left(\frac{\bar{\nu}_j(\boldsymbol{\kappa})}{2} \right) \delta\left(\epsilon' - \epsilon + \hbar\omega_j(\boldsymbol{\kappa})\right) + \right.$$
$$\left. + \left| \sum_{\mathbf{l}} e^{i(\mathbf{Q}-\boldsymbol{\kappa})\mathbf{l}} \right|^2 \left(\frac{\bar{\nu}_j(\boldsymbol{\kappa}) + 1}{2} \right) \delta\left(\epsilon' - \epsilon - \hbar\omega_j(\boldsymbol{\kappa})\right) \right], \tag{14}$$

where $\epsilon = \hbar^2 K^2/2m$ and $\epsilon' = \hbar^2 K'^2/2m$ are the initial and final values of the electron kinetic energy inside the crystal formed by N atoms, $\exp(-2W(Q))$ is the Debye–Waller factor, and $\bar{\nu}_j(\boldsymbol{\kappa})$ is the mean number of phonons. It is determined by the Bose–Einstein distribution

$$\bar{\nu}_j(\boldsymbol{\kappa}) = \left[\exp\left(\frac{\hbar\omega_j(\boldsymbol{\kappa})}{k_{\rm B}T} \right) - 1 \right]^{-1}. \tag{15}$$

Since the minimum electron kinetic energy $\epsilon \sim 10$ eV, while the maximum phonon energy $\hbar\omega \sim 0.1$ eV, one can neglect $\hbar\omega$ in the δ functions. Following Ziman [20], we consider only the so-called normal scattering of electrons without any diffraction. In addition, we approximate the phonon spectrum by the Debye model and believe that the sound velocity s is the same for all three branches of the acoustic vibrations. So that, we have

$$\omega_j(\boldsymbol{\kappa}) = \omega(\kappa) = s\kappa, \tag{16}$$

where the wave vector κ varies from 0 to the bound value $\kappa_{\mathcal{D}}$, given by [20]

$$\kappa_{\mathcal{D}} = \left(6\pi^2/v_0\right)^{1/3}. \tag{17}$$

The corresponding maximum frequency is

$$\omega_{\rm D} = k_{\rm B}\theta_{\rm D}/\hbar, \tag{18}$$

where $\theta_{\rm D}$ is the Debye temperature. These quantities determine the sound velocity:

$$s = \omega_{\rm D}/\kappa_{\mathcal{D}}. \tag{19}$$

In what follows, the average number of phonons $\bar{\nu}_j(\boldsymbol{\kappa})$ depending only on $|\boldsymbol{\kappa}|$ will be designated by $\bar{\nu}(\kappa)$.

Moreover, the Debye model yields

$$2W(Q) = \frac{3\hbar^2 Q^2 T^2}{M k_{\rm B}\theta_{\rm D}^3} \int\limits_0^{\theta_{\rm D}/2} \left[\frac{1}{e^z - 1} + \frac{1}{2}\right] z dz. \tag{20}$$

In (14), we first integrated over $\boldsymbol{\kappa}$ and after that over the spherical coordinates K', ϑ, ϕ of the vector $\mathbf{K}'$, using the equality

$$Q^2 = 2K^2 t, \quad t = 1 - \cos\vartheta. \tag{21}$$

Here, ϑ represents the angle between the wave vectors $\mathbf{K}'$ and $\mathbf{K}$.

Then the inelastic scattering cross section of electrons referred to one atom of the crystal,

$$\sigma_{\rm in} = \sigma_{\rm in}^{(N)}/N, \tag{22}$$

becomes

$$\sigma_{\rm in} = 4\pi\left(\frac{mZe^2 r_0^2}{\hbar^2}\right)^2 \times$$
$$\times \left(\frac{\hbar K}{Ms}\right) \int\limits_0^{t_{\rm max}} dt \frac{\sqrt{2t}e^{-2W(K\sqrt{2t})}}{(1 + 2K^2 r_0^2 t)^2}\left[\bar{\nu}(K\sqrt{2t}) + \frac{1}{2}\right], \tag{23}$$

where $t_{\rm max} = \kappa_{\rm D}^2/2K^2$.

3. Energy Spectrum

Let a crystal film be formed by N_p crystal planes spaced by distance d. They are numerated by the number $n = 0, 1, 2, ..., N_p - 1$, where the number $n = 0$ is associated with the plane on the face surface. The thickness of such a film equals $D = N_p d$.

The energy and angular distribution of shake-off electrons emitted from the crystal after the decay of a nucleus embedded in the n-th plane is described by a function $w_n(E,\theta)$, so that the average number of electrons emitted in the energy interval ΔE at a solid angle $\Delta\Omega$ after the decay of one nucleus in the n-th plane is

$$\Delta N_e^{(n)} = \int\limits_{\Delta E} dE \int\limits_{\Delta\Omega} d\Omega w_n(E,\theta). \tag{24}$$

This distribution is defined by the expression [18]

$$w_n(E,\theta) = w_0(E,\theta)\exp\left\{-\mu(E)nd/\cos\theta_0\right\}, \tag{25}$$

where $w_0(E,\theta)$ is the distribution of electrons ejected after the decay of a nucleus lying on the surface, θ_0 or θ is, respectively, the angle between the electron wave vector $\mathbf{K}$ or $\mathbf{k}$ and the z axis which is perpendicular to the surface of the crystal film. They are connected by the relation [18]

$$\cos\theta_0 = \left(1 - \frac{E}{E + U_0}\sin^2\theta\right)^{1/2}. \tag{26}$$

The distribution $w_0(E,\theta)$ written in terms of the dimensionless parameters

$$\tilde{K} = Kr_0, \quad \tilde{q} = qr_0, \tag{27}$$

has the form [18]

$$w_0(E,\theta) = T(E)\left(\frac{r_0}{a}\right)^5 \frac{1}{E_0}\sqrt{\frac{2E}{E_0}}\frac{8}{\pi^3} \times$$
$$\times \int\limits_0^{\tilde{q}_{\rm max}} \frac{\tilde{n}(\tilde{q})\tilde{q}^2 d\tilde{q}}{[\tilde{K}^2 - \tilde{q}^2][1 + 2(\tilde{K}^2 + \tilde{q}^2) + (\tilde{K}^2 - \tilde{q}^2)^2]}, \tag{28}$$

where $a = \hbar^2/me^2$ and $E_0 = e^2/a$ are the Bohr radius and the atomic unit of energy, respectively,

$$T(E) = \frac{4(1 + U_0/E\cos^2\theta)^{1/2}}{[1 + (1 + U_0/E\cos^2\theta)^{1/2}]^2} \tag{29}$$

is the transmission coefficient of an electron wave through the surface, and

$$\tilde{n}(\tilde{q}) = \left[\exp\left\{\frac{\alpha\tilde{q}^2 - \varepsilon_{\rm F}}{k_{\rm B}T}\right\} + 1\right]^{-1} \tag{30}$$

with

$$\alpha = \hbar^2/2mr_0^2 \tag{31}$$

represents the Fermi distribution for conduction electrons depending on the dimensionless parameter $\tilde{q}$.

The integration in (28) is performed over all bound states $|\mathbf{q}\rangle$ of the conduction electrons in the potential well with the depth U_0. Therefore, the upper limit of integration $\tilde{q}_{\rm max}$ in (28) should be taken a bit less than $\sqrt{2mU_0}r_0/\hbar$.

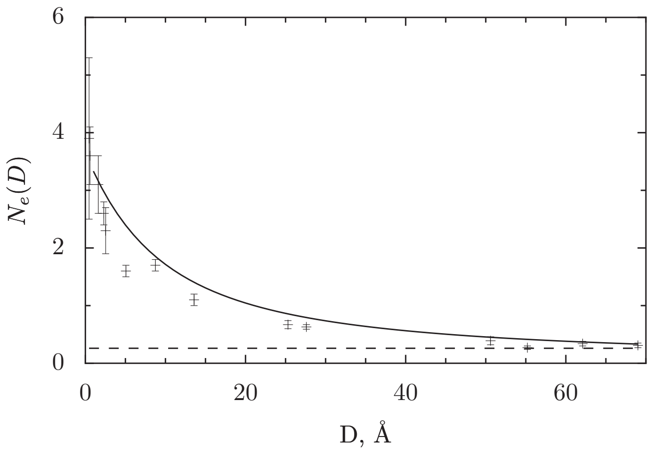

Fig. 1. Average yield of shake-off electrons N_e from a copper crystal after the single decay of a radioactive nucleus as a function of the crystal thickness D. Our calculations are drawn by the solid line, while the data of [16] are presented by dots. The dashed line indicates the experimental background

4. Yield of Electrons

By averaging (25) over all crystal planes, we get a distribution of shake-off electrons emitted from the slab after the single nuclear decay at any point of the crystal:

$$\overline{w(E,\theta)} = w_0(E,\theta)\frac{1}{N_p}\frac{1-e^{-\mu(E)D/\cos\theta_0}}{1-e^{-\mu(E)d/\cos\theta_0}}. \qquad (32)$$

For a thick crystal, when $\mu D \gg 1$, this expression is reduced to

$$\overline{w(E,\theta)} = w_0(E,\theta)\frac{1}{N_p}\frac{1}{1-e^{-\mu(E)d/\cos\theta_0}}. \qquad (33)$$

The energy distribution of all electrons emitted from the metal is determined by the integral over the angles:

$$W(E) = 2\pi\int\limits_0^{\pi/2}\overline{w(E,\theta)}\sin\theta d\theta. \qquad (34)$$

The average number of low-energy electrons ejected from the crystal following the decay of one nucleus located at an arbitrary point of the crystal is given by the integral

$$N_e = \int\limits_0^{\infty} W(E)dE + B, \qquad (35)$$

where B denotes any experimental background.

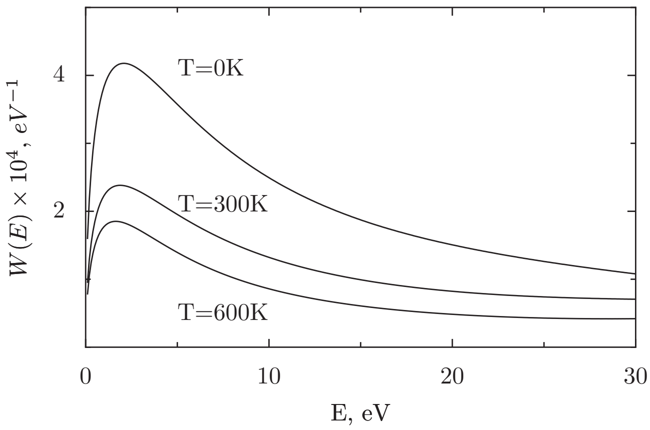

Fig. 2. Energy distribution of shake-off electrons emitted from a copper film at various temperatures

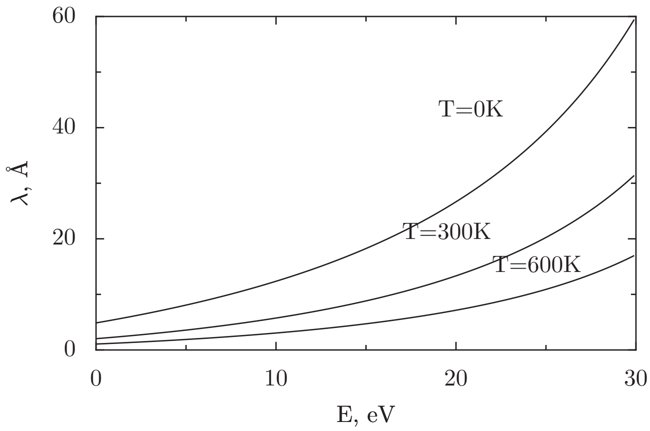

Fig. 3. Energy dependence of the free path length for electrons in a copper crystal at various temperatures

The number N_e of low-energy electrons emitted from a copper film as a function of the film thickness D has been recently measured in [16]. Such electrons escape mainly from the conduction band, since they are most weakly bound as compared with inner electrons of ions. We calculated the function $N_e(D)$, by using the following parameters for the copper film: $v_0 = 1.2\times 10^{-23}$ cm^3, $\varepsilon_F = 7.0$ eV, $A = 4.4$ eV, $\theta_D = 315$ K, $U_0 = 11.4$ eV, and $r_0 = 0.55$ Å. From Eqs. (32)–(35), one sees that the number of emitted shake-off electrons per one nuclear decay falls down with increase in N_p due to the attenuation of the electron wave inside the crystal. The attenuation coefficient has been calculated with the aid of Eqs. (5) and (23). Our results are compared with the experimental data in [16] in Fig. 1.

In addition, the energy distribution $W(E)$ for electrons emitted from a copper film is presented in Fig. 2

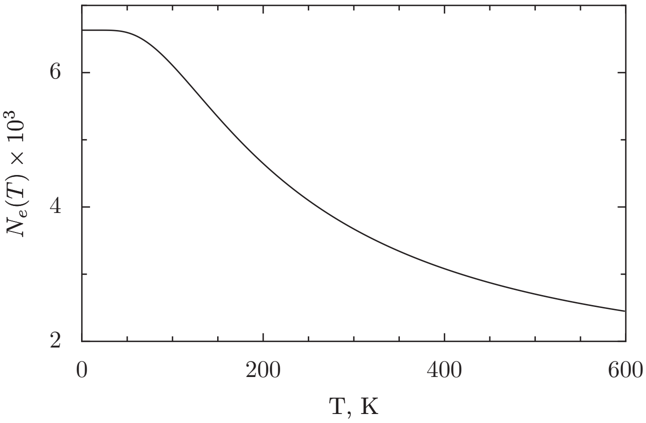

Fig. 4. Temperature dependence of the integral electron yield from a copper film

at the temperatures $T = 0$, 300, and 600 K. For definiteness, we took the number of crystal planes $N_p = 40$. We see that, as T grows, the shape of the curve $W(E)$ changes due to the strong dependence of μ on the energy E.

The energy dependence of the free path length $\lambda = \mu^{-1}$ for low-energy electrons in copper is displaced in Fig. 3 at the same temperatures. It is seen that λ decreases with increase in the temperature due to growing the average number of phonons and, respectively, the amplitude of vibrations.

The total yield of electrons N_e from the same copper film, as is shown in Fig. 4, decreases with increase in the temperature due to raising the attenuation μ of electron waves.

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ТЕМПЕРАТУРНА ЗАЛЕЖНІСТЬ ЕФЕКТУ СТРУСУ ЕЛЕКТРОНІВ ПРОВІДНОСТІ В МЕТАЛАХ

О.Я. Дзюблик, В.Ю. Співак

Р е з ю м е

Проаналізовано емісію із металу електронів провідності, спричинену ядерним розпадом. Враховано заломлення електронної хвилі на поверхні кристала та затухання, викликане розсіянням на фононах. Показано, що енергетичний розподіл випромінених електронів струсу має пік при енергії порядку 1 еВ, інтенсивність якого спадає зі зростанням температури. Вивчено також залежність виходу електронів провідності від товщини зразка.