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EMISSION OF CONDUCTIVITY ELECTRONS FROM METALS, PRODUCED BY IONS

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The number of conductivity electrons ejected from the metal foil by incident ions is calculated in the Born approximation. The interaction between the ion and electrons is approximated by the screened Coulomb potential. The conductivity electrons are treated as an ideal gas, confined in the potential well. Attenuation of the electron wave, excited by an ion inside the crystal, as well as its refraction at the crystal surface are taken into consideration.

Keywords: secondary electron emission, metal strip detectors, ions, conductivity electrons.

Introduction

For long time the bombardment of solids by ions attracts attention of both experimentalists and theorists due to numerous technical applications. Lately the problem of secondary electron emission became acute owing to construction of metal strip detectors [1], which are used for monitoring of ion beams at accelerators. Existing theories of inelastic scattering of charged particles by solids, leading to electron emission, consider mainly excitation of electrons bound in the isolated atoms (see, e.g., [2 - 5]). The questions about ejection of the conductivity electrons from the conductivity band in metals as well as the role of crystal environment remain beyond the scope of such approaches. All these questions are addressed in our paper. It will be done in analogy with our treatment [6, 7] of the shake-off process of conductivity electrons, provided either by β decay of the nuclei or by electron capture and internal conversion, which lead to abrupt alteration of the Coulomb field governing electrons. We shall take into consideration attenuation of the electron wave, to be excited by an ion moving through a crystal, as well as its refraction at the surface. Note that emission of loosely bound conductivity electrons is much more effective than that of deeply bound atomic electrons, since the inelastic scattering cross section quickly falls down with increasing energy transferred by a projectile to the target [4].

Basic equations

Let the crystal film have the thickness $D = L_3$ and transversal dimensions $L_1 \times L_2$. Its volume is $V_c = SD$, where $S = L_1 L_2$. Hereafter we put the origin of the coordinate frame x, y, z on the face surface of the film and direct axis z perpendicularly to it. The ions are incident from the region $z < 0$ perpendicularly to the surface with the wave vector $\boldsymbol{\kappa} = \{0, 0, \kappa\}$ and kinetic energy $\varepsilon(\kappa) = \hbar^2\kappa^2 / 2M$. The film is assumed to be very thin, so that the spreading of the ion beam over energies and angles due to collisions with nuclei of the target can be neglected.

In the metal the conductivity (valent) electrons, moving in a periodic crystal potential $U(r)$, are described by the Bloch wave functions. We shall use a simplified model, which treats electrons as free particles, moving in the rectangular potential well (see, e.g., [8])

$$U(r) = \begin{cases} -U_0 & \text{inside,} \\ 0 & \text{outside.} \end{cases} \quad (1)$$

The depth of this potential well equals

$$U_0 = E_F + A, \quad (2)$$

where $E_F = \hbar^2 q_F^2 / 2m$ is the Fermi energy and A is the work function. The radius of the Fermi sphere equals [8]

$$q_F = \left(3\pi^2 n_0\right)^{1/3}, \quad (3)$$

where n_0 is the concentration of the conductivity electrons:

$$n_0 = \frac{\nu}{\text{v}_0}, \quad (4)$$

v_0 is the volume of the elementary cell (we assume that it contains one atom), ν is the valency of the atoms. The electron wave vectors run the values $q_\alpha = \frac{2\pi}{L_\alpha} n_\alpha$, where $n_\alpha = 0, \pm 1, \pm 2, ...$ and $\alpha = x, y, z$. The same expression is valid for all other wave vectors inside the crystal.

The Hamiltonian of the system (ion + one conductivity electron) can be written down as

$$\hat{H}(\mathbf{r}, \mathbf{R}) = \hat{H}_0(\mathbf{r}, \mathbf{R}) + V(\mathbf{r}'), \quad (5)$$

where $\mathbf{r}$ and $\mathbf{R}$ are the radius-vectors of the electron and nucleus of the incident ion, respectively, $\mathbf{r}' = \mathbf{r} - \mathbf{R}$.

The unperturbed Hamiltonian

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + U(\mathbf{r}) - \frac{\hbar^2}{2M}\Delta_{\mathbf{R}}, \qquad (6)$$

where m and M are the electron and ion masses, respectively.

Let the ion charge be ΔZe and the charge of its nucleus be Ze. The Coulomb interaction of the incident ion with any electron of the target should be written in the form

$$V(r') = -\frac{Ze^2}{r'} g(r'), \qquad (7)$$

where $g(r')$ is the screening factor, which obeys the condition $g(0) = 1$. Outside the ion its potential coincides with the potential of the point charge ΔZe, screened by the cloud of free conductivity electrons, i.e.,

$$V(r') \approx -\frac{\Delta Ze^2}{r'} e^{-r'/r_0}, \qquad (8)$$

where the screening length r_0 is determined by the well known formula [8]

$$r_0 = \left(\frac{E_F}{6\pi e^2 n_0}\right)^{1/2}. \qquad (9)$$

For completely stripped ions the interaction $V(r')$ is described by Eq. (8) in the whole region $0 \le r' < \infty$. At the same time, inside the ion, the density of bound electrons, as a rule, much larger than the density of free electrons, and the screening is realized mainly by bound electrons. According to the Thomas - Fermi statistical model their distribution is characterized by the radius $r_a = a_0 Z^{-1/3}$ [5,9], where $a_0 = \hbar^2 / me^2$ is the Bohr radius of the atom. The screening factor $g(r')$, which satisfies all these constraints, can be written as

$$g(r') = \frac{Z'}{Z} e^{-r'/r_a} + \frac{\Delta Z}{Z} e^{-r'/r_0}, \qquad (10)$$

where $Z' = Z - \Delta Z$. Accordingly, the interaction $V(r')$ becomes

$$V(r') = -\frac{Z'e^2}{r'} e^{-r'/r_a} - \frac{\Delta Ze^2}{r'} e^{-r'/r_0}. \qquad (11)$$

The eigenfunctions and eigenvalues of the operator $\hat{H}_0$ are determined by equation

$$\hat{H}_0 \phi_b(\mathbf{r}, \mathbf{R}) = E_b \phi_b(\mathbf{r}, \mathbf{R}). \qquad (12)$$

We impose periodic boundary conditions on the frontiers of the crystal. Then the conductivity electrons, moving in the potential well (1), are described by the wave functions

$$\psi_{\mathbf{q}}(r) = \frac{1}{\sqrt{V_c}} e^{i\mathbf{qr}}. \qquad (13)$$

The corresponding energy will be

$$E(\mathbf{q}) = -U_0 + \hbar^2 q^2 / 2m. \qquad (14)$$

The initial state of the system is described by the product of the function (13) and plane wave to describe the ion:

$$\phi_a(\mathbf{r}, \mathbf{R}) = \frac{1}{\sqrt{V_c}} e^{i\mathbf{qr}} \frac{1}{\sqrt{V_c}} e^{i\kappa\mathbf{R}}. \qquad (15)$$

The average number of electrons on the level $\mathbf{q}$ with definite spin projection is determined by the Fermi distribution

$$\bar{n}(\mathbf{q}) = \left[\exp\left(\frac{E(\mathbf{q}) - E_F}{k_B T}\right) + 1\right]^{-1}. \qquad (16)$$

The electron flies away into the region $z > D$. In the final state ϕ_b the wave vector of the ion is $\boldsymbol{\kappa}'$, whereas the electron attributes the wave vector $\mathbf{K}$ inside the crystal and $\mathbf{k}$ outside it. The final electron energy

$$E(K) = -U_0 + \frac{\hbar^2 K^2}{2m} = \frac{\hbar^2 k^2}{2m}. \qquad (17)$$

As to the ion, we assume that its both initial $\varepsilon(\kappa)$ and final $\varepsilon(\kappa')$ energies much exceeds U_0, so that refraction of the ion wave on the surface is negligible. The energies of the system in the initial and final states will be

$$E_a = E(q) + \varepsilon(\kappa), \quad E_b = E(K) + \varepsilon(\kappa'). \qquad (18)$$

Emission of electrons

The transition probability per unit time, calculated in the Born approximation, is determined by

$$P_{a\to b} = \frac{2\pi}{\hbar} |V_{ba}|^2 \delta(E_b - E_a). \qquad (19)$$

Here the matrix element may be written as

$$V_{ba} = \frac{1}{V_c}\int e^{i(\mathbf{q}-\mathbf{K})\mathbf{r}'}V(r')d\mathbf{r}'\frac{1}{V_c}\int e^{i(\mathbf{Q}+\mathbf{q}-\mathbf{K})\mathbf{R}}d\mathbf{R}, \quad (20)$$

where $\mathbf{Q} = \boldsymbol{\kappa} - \boldsymbol{\kappa}'$ is the scattering vector of the ion. The integration over $\mathbf{R}$ within a finite volume of the crystal immediately gives the Kronequer symbol $\delta_{\boldsymbol{\kappa}+\mathbf{q},\,\boldsymbol{\kappa}'+\mathbf{K}}$, which expresses the momentum conservation law, from which it follows that

$$\mathbf{Q} = \mathbf{K} - \mathbf{q}. \quad (21)$$

It is convenient to write down these vectors in cylindrical coordinates:

$$\mathbf{q} = \{q_\parallel \cos\phi, q_\parallel \sin\phi, q_z\},$$

$$\mathbf{K} = \{K_\parallel \cos\phi', K_\parallel \sin\phi', K_z\}, \quad (22)$$

where $\mathbf{q}_\parallel$ and $\mathbf{K}_\parallel$ denote their projections on the plane x, y.

From inequality $m << M$ it follows that the velocity of heavy ion does not practically change during collision with a light electron, i.e., $Q << \kappa$. This inequality and condition (21) allows us to represent the delta function of Eq. (19) in the form

$$\delta(E_a - E_b) \approx \frac{m}{\hbar^2}\frac{1}{f(K_z)}\delta\left(K_\parallel - f\ (K_z)\right), \quad (23)$$

where we introduced the notation

$$f(K_z) = \left(q^2 + \frac{2m}{M}\kappa(K_z - q_z) - K_z^2\right)^{1/2}. \quad (24)$$

By summing (19) over $\boldsymbol{\kappa}$ and using the well-known matrix element for the screened Coulomb potential (see, e.g., [9]), one obtains the probability $P_{\mathbf{q}\to\mathbf{K}}$ for the electron transition per unit time inside the crystal from the state $\mathbf{q}$ to $\mathbf{K}$:

$$P_{\mathbf{q}\to\mathbf{K}} = \frac{2\pi}{\hbar^3}\frac{1}{V_c^2}\left(\frac{4\pi Ze^2}{Q^2 + \frac{1}{r_0^2}}\right)\frac{m}{f(\mathrm{K}_z)}\delta(K_\parallel - f(K_z)). \quad (25)$$

Collision of the incident ion with a conductivity electron can occur with equal probability in any volume element ΔV_c inside the crystal film. Therefore the unit time probability of the electron transition $\mathbf{q} \to \mathbf{K}$, occuring in the region from z to $z + \Delta z$, equals $P_{\mathbf{q}\to\mathbf{K}}(\Delta z / D)$. The electron wave, born in this interval, suffers attenuation when propagating towards the surface $z = D$. The main reason of such an attenuation is an inelastic scattering of the electron wave by vibrating ions of the crystal [8]. The intensity of the electron beam, which passed the distance x inside the crystal, decreases exponentially:

$$I(x) = I(0)e^{-x/l}, \quad (26)$$

where l is the mean-free path of the electrons. Its energy dependence is usually described with the aid of semi-empirical formulas, one of which reads [10]

$$l(E) = 538\tilde{a}\tilde{E}^{-2} + 0.41\tilde{a}^{3/2}\tilde{E}^{1/2}, \quad (27)$$

where $\tilde{E} = E / 1\,\mathrm{eV}$ and $\tilde{a}^3 = \mathrm{v}_0 / 1\,\mathrm{nm}^3$ with v_0 representing the volume per one atom (for crystals with single atom in the elementary cell v_0 is simply the elementary cell volume).

The conductivity electron, which attributed energy E' in the target layer $(z, z + \Delta z)$, will fly away from the crystal with the probability being equal to $exp\{(D - z) / l(E')\cos\theta_0\}T(K_z)$, where θ_0 is the angle between the vector $\mathbf{K}$ and the axis z, while $T(K_z)$ is the transmission coefficient of the electron wave from the crystal to the vacuum:

$$T(K_z) = \frac{4K_z k_z}{(K_z + k_z)^2}. \quad (28)$$

From the energy conservation law (17) and equality of the tangential components of the electron wave vectors inside ($\mathbf{K}_\parallel$) and outside ($\mathbf{k}_\parallel$) the crystal it follows that

$$k_z = \sqrt{K_z^2 - 2mU_0 / \hbar^2}. \quad (29)$$

So the probability of the electron ejection in the vacuum per unit time equals a product of all these probabilities summed over the crystal layers along the axis z from 0 to D:

$$P_{\mathbf{q}\to\mathbf{k}}^{out} = P_{\mathbf{q}\to\mathbf{K}}\frac{1}{D}\int_0^D dz e^{-(D-z)/l(E')\cos\theta_0}T(K_z). \quad (30)$$

The corresponding cross section, when the free path l is much less than the film thickness D, becomes

$$\sigma_{\mathbf{q}}(\mathbf{Q}) = \frac{1}{v}P_{\mathbf{q}\to\mathbf{K}}\frac{l(E')\cos\theta_0}{D}T(K_z), \quad (31)$$

where $v = \hbar\kappa / M$ is the velocity of incident ions.

This cross section should be yet averaged over all possible final states of the electron and summed over all electrons of the conductivity band. For this aim we pass from summation over **q** and **K** to integration:

$$\sum_{\mathbf{q}} \to \frac{V_c}{(2\pi)^3}\int d\mathbf{q}, \qquad \sum_{\mathbf{K}} \to \frac{V_c}{(2\pi)^3}\int d\mathbf{K}\,. \quad (32)$$

Integrating first (25) over $K_\parallel$, we remove the δ function. Then making use of the expression

$$Q^2 = K^2 + q^2 - 2q_\parallel f(K_z)\cos\alpha - 2q_z K_z \quad (33)$$

with $\alpha = \phi' - \phi$, we perform integration over α:

$$\int_0^{2\pi} \frac{d\alpha}{(a+b\cos\alpha)^2} = \frac{2\pi a}{(a^2-b^2)^{3/2}}. \quad (34)$$

Here the following dimensionless parameters are introduced:

$$a = 1 + [(q_z - K_z)^2 + K_\parallel^2 + q_\parallel^2]r_0^2, \quad b = -2K_\parallel q_\parallel r_0^2. \quad (35)$$

Integrating further over K_z one should keep in mind that only electrons with $K_z > \sqrt{2mU_0}/\hbar$ are able to overcome the potential barrier at the surface. The upper limit of such an integration K_2 follows from the evident requirement that $K_\parallel$ should be positive, i.e., $f(K_z) \ge 0$. Equating $f(K_z)$ to zero, one has the quadratic equation

$$K_z^2 - \frac{2m}{M}\kappa K_z + \frac{2m}{M}\kappa q_z - q^2 = 0, \quad (36)$$

whose roots are

$$K_z^{\pm} = \frac{m}{M}\kappa \pm \sqrt{\left(\frac{m}{M}\kappa\right)^2 - \frac{2m\kappa q_z}{M} + q^2}\,. \quad (37)$$

The function $f(K_z) > 0$, when $K_z^- < K_z < K_z^+$. Hence, the upper limit of integration $K_2 = K_z^+$. But it remains to choose the lower limit K_1, which is greater both numbers K_z^- and $\sqrt{2mU_0}/\hbar$. Note that K_z^- reaches its maximal value K when $\mathbf{q} = \{0,0,q\}$. But for the conductivity electrons bound in the crystal q always less than $\sqrt{2mU_0}/\hbar$. Therefore we must take $K_1 = \sqrt{2mU_0}/\hbar$.

Averaging over the initial states **q** of the conductivity band should be carried out within the sphere of the radius q_m, which contains all the electrons, i.e., $\bar{n}(q_m) \approx 0$. The only restriction for such a radius is that $q_m < \sqrt{2mU_0}/\hbar$, when the electrons are still bound in the crystal.

Thus, we arrive at the following expression for the integral cross section of the electron ejection, being produced by incident ions:

$$\sigma_e = \frac{3}{4\pi q_F^3}\int d\mathbf{q}\,\bar{n}(\mathbf{q})\sigma_{\mathbf{q}}, \quad (38)$$

where integration has to be done in the sphere of the radius q_m, the cross section $\sigma_{\mathbf{q}}$ characterizes the electron emission from the level **q**:

$$\sigma_{\mathbf{q}} = \frac{2\pi m}{v\hbar^3}(2Ze^2r_0^2)^2\int_{K_1}^{K_2} dK_z \frac{a}{(a^2-b^2)^{3/2}}\frac{l(E')\cos\theta_0}{D}T(K_z). \quad (39)$$

Numerical estimations show that with good accuracy at room temperature one can replace $\bar{n}(\mathbf{q})$ by unity at $0 \le q \le q_F$ and zero otherwise since $k_B T << E_F$. Therefore we replace q_m by q_F.

The flux of electrons emitted from the target is given by [11]

$$J_{out} = \sigma_e n_0 V_c j_0, \quad (40)$$

where j_0 is the flux density of incident ions. Accordingly, the number of electrons, knocked from a metal film by one ion $(j_0 = 1/S)$, is

$$\gamma = \sigma_e n_0 D. \quad (41)$$

Substituting here Eqs. (38), (39) and taking into account the above remarks one has finally

$$\gamma = \frac{3\pi m M}{(\hbar\kappa)(\hbar q_F)^3}(2Ze^2r_0^2)^2\int_{-q_F}^{q_F} dq_z \int_0^{\sqrt{q_F^2-q_z^2}} q_\parallel dq_\parallel \times$$

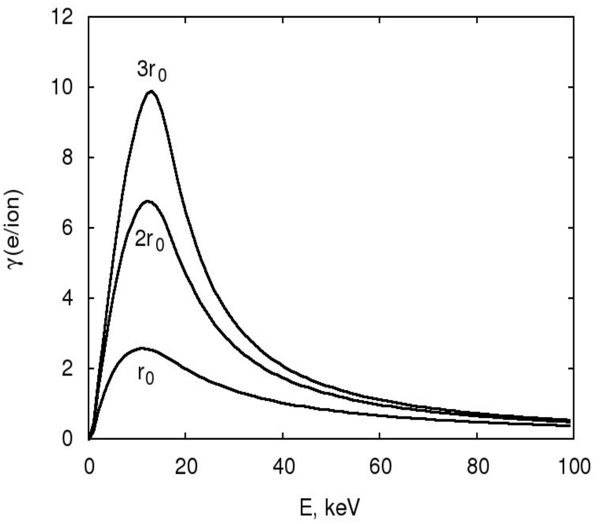
$$\times\int_{K_1}^{K_2} dK_z \frac{a}{(a^2-b^2)^{3/2}} l(E')\cos\theta_0 T(K_z) n_0 \quad (42)$$

with $\cos\theta_0 = K_z / K$.

Discussion

In our paper we analyzed emission of the conductivity electrons from metals bombarded by ions, taking for the first time into account spreading of these electrons over the levels of the conductivity band, corresponding to different energies and momenta. Moreover, we regarded the role of the electron screening of the coulomb interaction between incident ions and electrons of the target.

We performed numerical calculations of the electron yield produced by protons and deuterons incident on the golden film. The screening radius for point charge in the golden crystal has been calculated by means of the formula (9). It occurs to be equal 5.8 nm. For protons the results are presented in the Figure, when its energy ranges from 0 to 100 keV.



Dependence of the electron yield from Au on the energy of incident protons for different screening radii ($r_0 = 5.8$ nm).

The protons with such energies have velocities of the same order of magnitude as the conductivity electrons on the Fermi level. Therefore the electrons are able to follow moving protons. In other words, a proton entering the crystal gives rise to polarization of electrons in the conductivity band, which then moves together with the proton inside the crystal. As a result, polarized cloud of electrons screens the Coulomb field of the projectile. However, this screening may be more weak than that in the case of a stationary charge embedded in a crystal. Respectively, the screening radius becomes larger than r_0 given above. Therefore in the figure we displayed also the curves for the screening lengths $2r_0$ and $3r_0$. We see that the yield of secondary electrons quickly falls down with decreasing screening length. Such behavior has simple explanation. With lowering screening radius the attractive Coulomb potential of the ion narrows, that is its effective attraction weakens. Then the conductivity electron, moving relative to the ion, spends less time in this potential well, that leads to lowering of the kinetic energy transfer probability from the ion to electron (see also [12]).

Notice that the emission curves for deuterons and protons, when plotted as a function of their velocities, completely coincide in correspondence with the observations [3]. Magnitude of the secondary electron yield from Au by protons correlates with the experimental data [3], if we take the screening length somewhat larger than r_0. But calculated curve for the electron yield occurs to be narrower and shifted to lower energies compared to experimental curve. This may be explained as follows.

The formulas for the secondary emission coefficient γ were derived in the single-collision approximation, i.e., we have been assuming that the charged projectile collides with any electron of the target only one time. This can be fulfilled only for extremely thin films. Generally when passing a target the ion losses its energy in multiple collisions with nuclei and electrons as well as changes direction of its motion. The rate of such energy losses is characterized by so-called inelastic stopping power dE/dx, which must be inserted in equations for quantitative analysis of the experimental data.

This program will be realized later.

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ЕМІСІЯ ЕЛЕКТРОНІВ ПРОВІДНОСТІ З МЕТАЛІВ, СПРИЧИНЕНА ІОНАМИ

У борнівському наближенні пораховано кількість електронів провідності, вибитих з металічної плівки падаючими іонами. Взаємодія між іоном та електронами апроксимується екранованим кулонівським потенціалом. Електрони провідності трактуються як ідеальний газ у потенціальній ямі. Враховано затухання електронної хвилі, збудженої іоном всередині кристала, а також її заломлення на поверхні кристала.

Ключові слова: вторинна електронна емісія, металеві стріп-детектори, іони, електрони провідності.

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ЭМИССИЯ ЭЛЕКТРОНОВ ПРОВОДИМОСТИ ИЗ МЕТАЛЛОВ, ВЫЗВАННАЯ ИОНАМИ

В борновском приближении вычислено количество электронов, излученных из металлической пленки под действием падающих ионов. Взаимодействие между ионом и электронами апроксимируется экранированным кулоновским потенциалом. Электроны проводимости трактуются как идеальный газ в потенциальной яме. Учтено затухание электронной волны, возбужденной ионом всередине кристалла, а также ее преломление на поверхности кристалла.

Ключевые слова: вторичная электронная эмиссия, металлические стрип-детекторы, ионы, электроны проводимости.

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