Generalized formula for electron emission taking account of the polaron effect

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Abstract. A generalized formula is derived for the electron emission current as a function of temperature, field, and electron work function in a metal–dielectric system that takes account of the quantum nature of the image forces. In deriving the formula, the Fermi–Dirac distribution for electrons in a metal and the quantum potential of the image obtained in the context of electron polaron theory are used.

1. Introduction

It is well known that, if a cathode is not specially purified, the most probable sites for the development of vacuum breakdown are nonmetallic inclusions conventionally present on the cathode surface (island-type or solid dielectric films, adsorbed atoms, etc) [1]. Emission processes involving these nonmetallic inclusions lead to the formation of so-called cathode spots of type 1, which are short-lived sources of plasma expanding into the electrode gap [1, 2]. In many cases, the operation of type 1 spots governs the development of a vacuum breakdown at the initial stage. The problem of correct description of emission processes involving nonmetallic inclusions is even more relevant to investigating the initial stage of a high-voltage discharge in a gas medium [3] as surface inclusions of this type are inevitable in the presence of gas.

We consider the emission processes occurring in a metal-cathode–adsorbed-nonmetallic-film–vacuum (gas medium) taking account of the electron polaron effect (figure 1). As shown previously in [4, 5], the interaction of an electron with the induced polarization of a dielectric medium affects the shape of the potential barrier that exists at the surface of a metal during electron emission.

2. Statement of the problem

The density of the emission current flowing through the potential barrier at a metal–vacuum (dielectric medium) interface can be described as [6]

\[ j(E, T) = e \int_{-\infty}^{\infty} N(W, T) D(W, T) dW, \]  

(1)

where \( j(E, T) \) is the emission current density, \( e \) is the electron charge, \( E \) is the applied electric field, \( T \) is the temperature of metal, and \( D(W, E) \) is the penetrability of the potential barrier at the cathode surface.
In the Sommerfeld model, the number of incident electrons per unit area per second is described by the formula

$$N(W, T) = \frac{4\pi mk_0 T}{h^3} \ln \left[ 1 + \exp \left( -\frac{W - W_F}{k_0 T} \right) \right],$$

(2)

where $W_F$ is the Fermi energy of the metal; $k_0$ and $h$ are Boltzmann’s and Plank’s constant, respectively, and $m$ is the effective electron mass.

The energy is counted from zero for a free electron outside the metal (figure 2); therefore, the electronic work function ($\Phi$) equals the Fermi energy:

$$W(x) = \frac{p^2(x)}{2m} + W_i(x),$$

(3)

where $p(x)$ is the momentum of the electron moving along the normal, and $W_i(x)$ is the effective potential energy of the electron (see figure 2) given by

$$W_i(x) = \begin{cases} W_e(x) - eEx, & x \geq 0, \\ -W_a, & x < 0. \end{cases}$$

(4)

Here, $W_e(x)$ is the quantum potential energy of the interaction of the electron with the fast polarization it induces at the metal–dielectric interface (in the limit, it becomes the classical image potential at $x \gg R_p$, where $R_p = [\hbar/(2m\omega_p)]^{1/2}$ is the electron polaron radius).

In the study [6] and in the subsequent theories, for the potential $W_e(x)$ the classical potential of image forces was used which has a singularity at $x = 0$, that is, it is incorrect both immediately at and near the interface ($x \sim R_p$).

### 3. Derivation of a generalized formula for electron emission

A general expression for quantum image potential $W_e(x)$ which describes the interaction of an electron with the fast polarization it induces (plasmons of valence electrons) at a metal–dielectric interface is given in [4, 5]. This expression, in view of its complexity, is difficult to use in calculations. However, it has been demonstrated [5, 7, 8] that the potential energy $W_e(x)$ can be approximated quite accurately by the expression

$$\tilde{W}_e(x) \approx -\frac{e^2}{(4x + x_0)\varepsilon},$$

(5)
Figure 2. Potential energy $W(x)$ of an electron near the surface of a metal at $x \geq 0$. Here, $W_i(x)$ is the classical image potential of the electron, $W_e(x)$ is the quantum potential of the interaction of the electron with the fast polarization it induces, $W(E) = -eEx$ is the potential energy of the electron–field interaction, $W_a$ is the effective potential energy of an electron inside the metal (constant quantity), $\Phi = W_F$ is the work function (equal to the Fermi energy), and $W_{tm}$ is the maximum value of $W_t(x)$; $W_e(0) = W_e(x = 0)$.

Here, $x_0$ is a parameter which coincides in order of magnitude with the electron polaron radius $R_p$. For typical parameter values, we have $m = (0.1–1)m_0$, and $R_p \sim (1–10) \times 10^{-8}$ cm; that is, the electron polaron radius ranges from one to several lattice constants.

Note that previously [7–9], the parameter $x_0$ was introduced in the classical image potential as a “cutoff factor” to eliminate the “unphysical divergence” at the surface of a crystal ($x = 0$).

For the penetrability $D(E, W)$ of the barrier at the interface, we can write:

$$D(E, W) = \left[ 1 + \exp \left( -\frac{4\pi i}{\hbar} \int_{x_1}^{x_2} p(x)dx \right) \right]^{-1},$$  

(6)

where $p(x)$ is the coordinate-dependent momentum of the emitted electron,

$$p(x) = \sqrt{2m(W - W_t(x))},$$  

(7)

$W_t(x)$ is the electron potential energy, which, in view of equations (3)–(5), can be determined as

$$W_t(x) = -\frac{e^2}{16\pi \varepsilon_0 \varepsilon (x + x_0/4)} - eEx.$$  

(8)

Thus, we have

$$p(x) = \sqrt{2m \left( W + \frac{e^2}{16\pi \varepsilon_0 \varepsilon (x + x_0/4)} \right) + eEx}.$$  

(9)
Equations (6)–(9) are written in accordance with SI units. The limits of integration in (6) are evaluated from the condition \( p(x) = 0 \). Then, in view of (9), we have
\[
W + \frac{e^2}{4\pi\varepsilon_0\varepsilon(x + x_0/4)} + eEx = 0. 
\]
To put the integral in (6), which involves (10), in the form considered in [6], we make the change of variable \( z = x + x_0/4 \). Then equation (10) can be rewritten as
\[
W(1 - \frac{eEx_0}{4W}) + \frac{e^2}{16\pi\varepsilon_0\varepsilon z} + eEz = 0. 
\]
Next, we introduce the notation used in [7]:
\[
\gamma = 1 - \frac{eEx_0}{4W}. 
\]
To evaluate the integration limits, we obtain from (10) a quadratic equation whose solution is:
\[
z_{1,2} = \frac{-\gamma W}{2eE} \pm \sqrt{\frac{\gamma^2 W^2}{4e^2E^2} - \frac{e}{16\pi\varepsilon_0\varepsilon E}}. 
\]
Introducing a new variable:
\[
y_a = \frac{e}{2|\gamma W|} \sqrt{\frac{eE}{\pi\varepsilon_0\varepsilon}} 
\]
and assuming that the energy \( W \) takes only negative values, we can write:
\[
z_{1,2} = \frac{-\gamma W}{2eE} \left(1 \pm \sqrt{1 - y_a^2}\right). 
\]
In view of the above notation, the integral in (6) becomes:
\[
I = -\frac{2\sqrt{2m}}{h} \int_{z_{2}}^{z_{1}} \left(\gamma W + \frac{e^2}{16\pi\varepsilon_0\varepsilon z} + eEz\right)^{1/2} dz. 
\]
The resulting integral is similar to that obtained in [8]. Integration of (16) yields a tabulated function \( \nu_a(y_a) \) as:
\[
\nu_a(y_a) = \sqrt{1 + \frac{1 - y_a^2}{2}} \left\{ E\left[\sqrt{\frac{2\sqrt{1 - y_a^2}}{1 + \sqrt{1 - y_a^2}}} - \left(1 - \sqrt{1 - y_a^2}\right) K\left[\frac{2\sqrt{1 - y_a^2}}{1 + \sqrt{1 - y_a^2}}\right]\right] \right\}, 
\]
where
\[
K[k] = \int_{0}^{\pi/2} \frac{d\theta}{\sqrt{1 - k^2 \sin^2 \theta}}, 
\]
\[
E[k] = \int_{0}^{\pi/2} \sqrt{1 - k^2 \sin^2 \theta} d\theta, 
\]
are an Euler beta and an Euler gamma integral, respectively.

Note that the function (17) is different from the Nordheim function [6] by the polaron term in the argument \( y_a \). Following Modinos [9], for the case \( y_a \leq 1 \) (which corresponds to the field emission mode), we obtain from (17):
\[
\nu_a(y_a) = \sqrt{1 + y_a} \left\{ E\left[\sqrt{\frac{1 - y_a}{1 + y_a}} - y_a K\left[\frac{1 - y_a}{1 + y_a}\right]\right] \right\}. 
\]
Figure 3. Function $\nu_a(y)$ for different values of factor $\gamma$.

The argument $y_a$ can be defined in terms of the argument $y$ of the Nordheim function as:

$$y_a = \frac{y}{\sqrt{\beta}}.$$  

Then, using (20), we obtain for $\nu_a(y)$ (assuming that $\varepsilon \approx 1$, which holds for the thickness of an adsorbed film on the nanosecond scale) the following expression:

$$\nu_a(y) = \sqrt{\frac{\gamma + \sqrt{\gamma^2 - y^2}}{2\gamma}} \left\{ \frac{2\sqrt{\gamma^2 - y^2}}{\gamma + \sqrt{\gamma^2 - y^2}} - \frac{\gamma - \sqrt{\gamma^2 - y^2}}{\gamma} K\left[ \frac{2\sqrt{\gamma^2 - y^2}}{\gamma + \sqrt{\gamma^2 - y^2}} \right] \right\}. \quad (21)$$

The function $\nu_a(y)$ is plotted in figure 3.

Accordingly, the total current through the interface is determined by the following expression

$$j(E, T) = k_0 T \int_{-W_a}^{W_m} \ln \left[ 1 + \exp\left( -\frac{W-W_F}{k_0 T} \right) \right] \frac{dW}{1 + \exp\left( \frac{1}{4} \sqrt{2E - 1/2y - 3/2\nu(y)} \right)}. \quad (22)$$

Expression (22) is written, like the formula in [6], in terms of Hartree units; that is $j$ is expressed in units of $m^3 e^9 \hbar^{-1} = 2.37 \times 10^9$ A/cm²; $E$ in units of $m^2 e^5 \hbar^{-1} = 5.15 \times 10^9$ V/cm; $W_F$, $k_0 T$, $W$, $W_a$, and $W_m$ in units of $m e^4 \hbar^2 = 27.2$ eV.

For high temperatures, at which the emission current is due to electrons overcoming a potential barrier of energy higher than $W_m$, integration (22) yields a formula for the polaron thermionic current density, which can be interpreted as a generalization of the Richardson–Schottky equation:

$$j_{RS}(E, T) = \frac{4\pi e m k_0^2}{\hbar^3} T^2 \exp \left[ -\frac{1}{k_0 T} \left( \frac{\Phi + eE x_0}{4\varepsilon} - \frac{1}{\varepsilon} \sqrt{\frac{e^3 E}{\pi}} \right) \right]. \quad (23)$$

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Integration in (22) in view of (16) and (20) yields an equation similar to the Murphy–Good formula [6]:

\[
    j(E, T) = \frac{e^3 E^2}{8 \pi h^2 e^{2\Phi} t_a(y)} - \frac{\pi c_a(y) k_0 T}{\sin (\pi c_a(y) k_0 T)} \exp \left[ -\frac{8 \pi e \Phi^{3/2} \sqrt{2m}}{3 e h E} \nu_a(y) \right].
\]

(24)

The tabled functions \( t_a(y) \) and \( c_a(y) \), which involve polaron contributions:

\[
    t_a(y) = \sqrt{\frac{\gamma \sqrt{\varepsilon} + y}{\gamma \sqrt{\varepsilon}}},
\]

\[
    c_a(y) = \frac{4 \pi \varepsilon \sqrt{2m} \Phi}{e h E} t_a(y).
\]

Here, the following designations are used:

\[
    y = \frac{e}{\gamma \Phi} \frac{E}{\sqrt{\varepsilon}}, \quad \gamma = 1 - \frac{e E x_0}{4 \Phi}.
\]

Equation (24) may be considered a generalized formula for the thermo-field-emission current density at a metal–adsorbed-nonmetal-nanofilm–vacuum contact, which takes into account the contribution of the polaron effect and its increase with electric field and temperature. It differs from the formula for emission current density derived by Murphy and Good [6] by the polaron contribution of the polaron effect and its increase with electric field and temperature. It differs from the formula for emission current density derived by Murphy and Good [6] by the polaron contribution involved in the arguments of the tabled functions \( \nu_a(y) \), \( t_a(y) \) and \( c_a(y) \).

For low temperatures \( (T \rightarrow 0) \), equation (24) yields a formula for the polaron field-emission current density, which can be interpreted as a generalization of the Fowler–Nordheim equation for cold electron emission:

\[
    j_{FN}(E) = \frac{e^3 E^2}{8 \pi h^2 e^{2\Phi} t_a^2(y)} \exp \left[ -\frac{8 \pi e \Phi^{3/2} \sqrt{2m}}{3 e h E} \nu_a(y) \right].
\]

(28)

Let us discuss the contribution of the polaron effect to the electron emission using of the equations (23) and (28) derived for the limiting cases. For fields \( E < 10^6 \) V/cm, the polaron effect is marginal so that an electron can be considered a classical particle, and both the Richardson–Schottky and the Fowler–Nordheim formula provide good agreement with experiment. For fields \( E > 5 \times 10^6 \) V/cm, at which the width of the potential barrier is comparable to the radius of an electron polaron, the wave properties of the electron becomes important and the polaron contribution to the emission current density becomes appreciable. This contribution is described by a parameter \( x_0 \) related to the radius of the electron polaron (tunneling quasi-particle).

An increase in polaron effect with electric field, on the one hand, increases the pure field emission current [see equation (28)] due to the presence of the function \( \nu_a(y) \) in the exponential (see figure 3) and, on the other hand, decreases the thermionic current [see equation (23)] due to an increase in effective work function \( \Phi = \Phi + e E x_0/(4\varepsilon) \). Which of the effects will prevail depends on specific experimental conditions.

4. Conclusion
A general formula for the emission current from a metal cathode having nonmetal inclusions has been derived taking into account the polaron effect. In the limiting cases, the formula becomes the Richardson–Schottky equation for thermionic emission or the Fowler–Nordheim equation for field emission. Subsequently, it is intended to analyze in detail the contribution of the polaron effect to the electron emission from metal cathodes for specific experimental conditions.

Acknowledgments
This work was supported in part by the Russian Foundation for Basic Research (grants No. 16-08-00604, 17-08-01282).
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