Limiting Field Emission Current Issue with the Quantum Image Forces

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***Abstract* — Relationships inherent in the processes that occur at the initial stage of a high-voltage (electric field strength $E > 1\ \mathrm{MV/cm}$) gas discharge with participation of nonmetal nanofilms adsorbed to the cathode are considered. It is shown that the current-voltage characteristic of the pre-breakdown current obeys the Fowler–Nordheim equation corrected for the quantum character of image forces. Based on electronic polaron theory, a general expression for the field emission current at the contact of between two media is obtained. It is shown that for the above-mentioned fields, the field dependence of the tunnel current is appreciably different from the well-known classical relations.**

***Key Words* — Nano layers, field emitter arrays, high-voltage gas discharge, polaron.**

I. Potential Energy Of An Electron In Adsorbed Dielectric Nanofilm

In our previous calculations of the current density of pre-breakdown field emission in a high-voltage discharge [1], we took into account the clusters of atoms or molecules adsorbed to the cathode. In gas discharges, adsorbates can form continuous films on the cathode surface. Precision experimental investigations of field and photostimulated field emission in metal–dielectric–semiconductor (MDS) structures have revealed a discrepancy between experiment and theory (Fowler–Nordheim equation) at high fields (over) [2–4]. For this reason, it is of interest to extend the theory (see, e.g., [5]) for the range of fields where image forces show a quantum behavior.

We consider a contact between a metal occupying a semi-infinite half-space and a tunnel thin dielectric film of permittivity. For the case of an external electric field of strength applied to the structure, the potential energy of an electron in the dielectric at the metal–dielectric interface is given by the expression

$$W(x) = W_F + \varphi + W_{ie}(x) - eEx, \quad x > 0, \tag{1}$$

where W_F is the Fermi energy counted from the bottom of the metal conduction band, φ is the work function, $W_{ie}(x)$ is the electronic part of the quantum potential of the image forces, and e is the elementary charge.

The emission current can be calculated by the expression for $W_{ie}(x)$ [6] derived based on the polaron theory [6–7] that is a generalization of Toyozawa's electronic polaron theory [8–9] for the case of a semi-bounded crystal with spatially dispersed permittivity. The expression obtained in Ref. 7 can be approximated by a simple formula:

$$W_{ie}(x) \approx -\frac{e^2}{\varepsilon(4x + x_0)}, \tag{2}$$

where ε is the permittivity of the adsorbed film, which can range from unity to the value of ε characteristic of a bulk sample of the given material, and x_0 is the interpolation parameter determined from the condition of between the asymptotic value of $W_{ie}(x)$ found from the approximate expression (2) and its exact value [8] in the limit $x \to 0$.

Numerical analysis has shown that the quantity x_0 can be approximated, to within $1-3\%$ for the actual range of x_0 values, by the expression

$$x_0 = \frac{2\left[1-(R_S/R_F)^2\right]e^2}{\pi\alpha_{pS}\hbar\omega_{pS}\left[1+(R_S/R_F)+2(R_S/R_F)^2\right]} \tag{3}$$

where $\hbar$ is the reduced Planck's constant (Dirac constant), R_F is the Fermi radius, $R_S = \left(\hbar\omega_{pS}/2m\right)^{1/2}$, m is the effective mass of an electron in the dielectric, $\omega_{pS} = \omega_{pV}/\sqrt{\varepsilon}$ is the frequency of the surface oscillation for the dielectric film–vacuum interface, ω_{pV} is the frequency of the longitudinal volumetric plasma oscillation of valence electrons, and

$$\alpha_{pS} = \frac{e^2}{\hbar}\left(1-\frac{1}{\varepsilon+1}\right)\left(\frac{m}{2\hbar\omega_{pS}}\right)^{1/2} \tag{4}$$

is a constant for the electron–plasmon interaction.

II. Curent Density Of The Field Emission Through Adsorbed Nonmetal Film

The following rearrangements are performed in the sequence used in Ref. 5, where the current density of the emission from a metal into a dielectric is calculated in terms of the Sommerfeld model as

$$j(F,T)=\int_0^{\infty} N(W,W_F,T)D(W,E)dW \ , \qquad (5)$$

where $W=W(x)$ is the energy of an electron counted from the conduction band bottom; $D(W,E)$ is the probability that an electron will penetrate the barrier, calculated in a semiclassical approximation; $N(W,W_F,T)$ is the number of electrons of energy close to W that are incident on the barrier per unit area in a second, and T is the absolute temperature.

$$D(W,E)=\left[1+\exp\left(-2i\int_{x_1}^{x_2}\lambda(x)dx\right)\right]^{-1}, \qquad (6)$$

$$\lambda(x)=\left(\frac{2m}{\hbar^2}\right)\left(W-W_F-\varphi-W_{ie}(x)+eEx\right)^{1/2} , \qquad (7)$$

$$N(W,W_F,T)=\frac{4\pi mkT}{h^3}\ln\left\{1+\exp\left[-\frac{W-W_F}{kT}\right]\right\} . \qquad (8)$$

Here k is Boltzmann's constant and $h=2\pi\hbar$ is Planck's constant.

Substituting (7) and (8) in (6) and performing integration, we obtain

$$D(W,E)=\left[1+\exp\left(\frac{4}{3}\sqrt{2}\left(\frac{E\hbar^4}{m^2e^5}\right)^{-1/4}y^{-3/2}v_a(y_a)\right)\right]^{-1} . \qquad (9)$$

The function $v_a(y_a)$ is an analog of the Nordheim function. It is tabulated by using the following expression, derived in view of an adsorbed film present on the emitter, which contains elliptic integrals $K[k]$ and $E[k]$ of the first and the second order, respectively:

$$v_a(y_a)=\gamma\sqrt{\frac{\gamma+a}{2}}\left(E\left[\sqrt{\frac{2a}{\gamma+a}}\right]-\left(\frac{\gamma-a}{\gamma}\right)K\left[\sqrt{\frac{2a}{\gamma+a}}\right]\right), \qquad (10)$$

where

$$\gamma=1-\frac{Ex_0}{4\varepsilon},. \quad y_a=\frac{1}{\phi}\sqrt{\frac{e^3E}{\varepsilon}}, \quad a=\sqrt{\gamma^2-y_a^2} . \qquad (11)$$

The main difference of $v_a(y_a)$ from the well-known Nordheim function is that its argument contains the parameters x_0 and ε that are characteristics of the potential barrier. The limiting electron energy, W_l (energy at the point of maximum of the potential barrier) is determined by the expression

$$W_l=-\left(\frac{e^3E}{2\varepsilon}+\left(\frac{eEx_0}{16}\right)^2\right)^{1/2}+\frac{eEx_0}{16} . \qquad (12)$$

The total current through the metal–dielectric interface is determined in Hartree units as

$$j_a=\frac{kT}{2\pi^2}\int_{-W_0}^{W_l}\frac{\ln\left\{1+\exp\left(-\frac{W-\varphi}{kT}\right)\right\}}{1+\exp\left(\frac{4}{3}\sqrt{2}E^{-1/4}y_a^{-3/2}v_a(y_a)\right)}dW$$

$$+\frac{kT}{2\pi^2}\int_{W_l}^{\infty}\ln\left(1+\exp\left(-\frac{W-\varphi}{kT}\right)\right)dW , \qquad (13)$$

where the lower limit of the first integral is the electron energy at the bottom of the metal conduction band.

With the criteria derived in Ref. 5, relation (13) yields, in the approximation of low temperatures, the formula for the field emission current density

$$j_a=\frac{E^2}{16\pi^2\phi\varepsilon^2t_a^2(y_a)}\exp\left(-\frac{4\sqrt{2}\,\varepsilon\phi^{3/2}}{3E}v_a(y_a)\right), \qquad (14)$$

where the effective work function ϕ depending on parameter x_0 is calculated by the formula

$$\phi=\varphi+\frac{x_0}{3}\left(E+\frac{E^2}{2\varepsilon}\right). \qquad (15)$$

The function $t_a(y_a)$ in the pre-exponential factor can also be expressed in terms of elliptic integrals:

$$t_a(y_a)=\gamma\sqrt{\frac{y_a}{2}}\left(2E\left[\sqrt{\frac{y_a-\gamma}{2y_a}}\right]-K\left[\sqrt{\frac{y_a-\gamma}{2y_a}}\right]\right). \qquad (16)$$

Expression (15) is a generalized Fowler–Nordheim formula represents for the field emission current which takes into account the quantum behavior of the image forces.

III. Computational Formulas

Using the coefficients relating the Hartree units to conventional units of physical quantities, we can obtain more

convenient and practical formulas. In this case, we must use the following multiplying factors of current density, electric field strength, and energy, respectively:

$$m^3e^9\hbar^{-7} = 2.37\times10^{14}\ \mathrm{A/cm^2},$$

$$me^4\hbar^{-2} = 27.2\,\mathrm{eV},$$

$$m^2e^5\hbar^{-4} = 5.15\times10^3\ \mathrm{MV/cm}.$$

If necessary, a factor $4\pi\varepsilon_0$, where ε_0 is the electric constant, is also used.

Then formula (14) becomes

$$j_a = \frac{e^3E^2}{8\pi h\phi\varepsilon^2}\exp\left(-\frac{8\pi\varepsilon\sqrt{2m\phi^3}}{3ehE}v_a(y_a)\right). \qquad (17)$$

For the effective work function ϕ we obtain from (15)

$$\phi = \varphi + \frac{ex_0E}{3}\left(1+\frac{2\varepsilon_0^3h^4E}{\pi\varepsilon m^2e^5}\right). \qquad (18)$$

Substituting numerical values of the universal constants expressing the parameter x_0 in nanometers, we have from (18) the computational formula

$$\phi = \varphi + 0.033x_0E\left(1+9.61\times10^{-5}\frac{E}{\varepsilon}\right). \qquad (19)$$

Obviously, for the field range under consideration (up to $100\ \mathrm{MV/cm}$) and actual values of x_0 of the order of tenths of a nanometer, the second bracketed term can be neglected. Then we have

$$\phi = \varphi + \frac{ex_0E}{3} \quad \text{or} \quad \phi = \varphi + 0.033x_0E. \qquad (20)$$

The argument y_a of the tabulated function $v_a(y_a)$ is calculated by the formulas

$$y_a = \frac{e}{2\phi}\sqrt{\frac{eE}{\pi\varepsilon_0\varepsilon}} \quad \text{or} \quad y_a = \frac{0.379}{\phi}\sqrt{\frac{E}{\varepsilon}}. \qquad (21)$$

For the coefficient γ it is necessary to use the expressions

$$\gamma = 1-\frac{\varepsilon_0^2h^2Ex_0}{\varepsilon me^3} \quad \text{or} \quad \gamma = 1-9.2\times10^{-4}\frac{Ex_0}{\varepsilon}. \qquad (22)$$

As with the Fowler–Nordheim equation, the function $t_a(y_a)$ is slightly different from unity. In this case, we have from (17)

$$j_a = \frac{e^3E^2}{8\pi h\varepsilon^2\varphi\left(1+ex_0E/3\varepsilon\varphi\right)}$$

$$\times\exp\left(-\frac{8\pi\varepsilon\sqrt{2m\left(\varphi+ex_0E/3\right)^3}}{3ehE}v_a(y_a)\right). \qquad (23)$$

The use of relations (20)–(23) results in the final computational formula for the current density of field emission from a metal coated with a nonmetal nanolayer ($\varepsilon\approx1$) of adsorbed atoms or molecules

$$j_a = \frac{1.4\times10^6E^2}{\varphi\left(1+0.033x_0E/\varphi\right)}$$

$$\times\exp\left(-68.5\frac{\varepsilon\left(\varphi+0.033x_0E\right)^{3/2}}{E}v_a(y_a)\right). \qquad (24)$$

Let us compare the current density values obtained by using (24) with those resulting from the well-known Fowler–Nordheim equation for a clean metal surface

$$j = \frac{e^3E^2}{8\pi h\varphi}\exp\left(-\frac{8\pi\sqrt{2m\varphi^3}}{3ehE}v(y)\right), \qquad (25)$$

where

$$y = \frac{e}{2\varphi}\sqrt{\frac{eE}{\pi\varepsilon_0}} \quad \text{or} \quad y = 0.379\frac{\sqrt{E}}{\varphi}. \qquad (26)$$

For the actual work function and electric field strength ranges ($\varphi > 3.8$ eV, $E < 100\ \mathrm{MV/cm}$), the parameter y is no greater than unity. For this case [5], the function $v(y)$, like the earlier introduced function $v_a(y_a)$, can be expressed in terms of elliptic integrals:

$$v(y) = \sqrt{1+y}\left(E\left[\sqrt{\frac{1-y}{1+y}}\right]-yK\left[\sqrt{\frac{1-y}{1+y}}\right]\right). \qquad (27)$$

As a result, the ratio of the density of the current from a smooth metal surface coated with a nanolayer of adsorbed

atoms or molecules to that of the current from a pure surface is determined as

$$j_a = \frac{e^3 E^2}{8\pi h\varepsilon^2 \left(\varphi + ex_0 E/3\right)}$$

$$\times \exp\left(- \frac{8\pi\varepsilon\sqrt{2m\left(\varphi + ex_0 E/3\right)^3}}{3ehE} v_a(y_a) \right). \qquad (28)$$

The computational formula is

$$\frac{j_a}{j} = \frac{\varphi}{\left(\varphi + 0.033 x_0 E\right)}$$

$$\times \exp\left(- 68.5 \frac{\varepsilon\left(\varphi + 0.033 x_0 E\right)^{3/2}}{E} v_a(y_a) \right). \qquad (29)$$

The ratio j_a/j is presented in Fig.1 as a function of the applied electric field strength for different values of the work function φ.

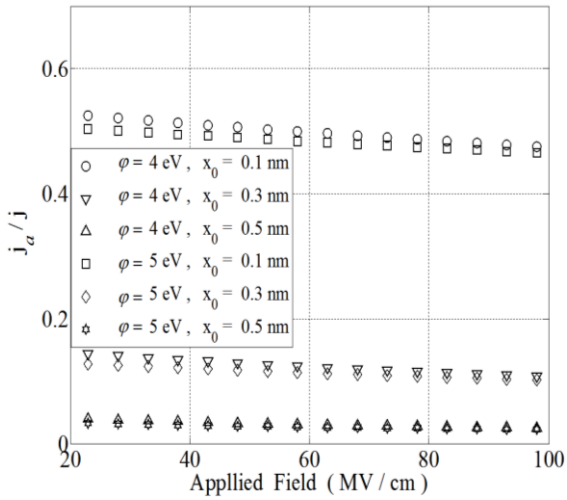

Fig. 1. The ratio of current density j_a to that of the field emission current from a clean metal surface *versus* electric field strength *E* for different values of work function φ.

CONCLUSIONS

1. Figure 1 shows an appreciable decrease in field emission current for all values of the parameter. It is of interest that the difference between and is less pronounced for the lower fields.

2. The rather weak dependence on the work function of the base cathode material is worthy of notice.

3. The field emission current noticeably decreases with parameter [quasiparticle (electronic polaron) radius]; that is, the quantum behavior of the image forces is pronounced in strong electric fields.

4. The variations in the work function of the cathode material due to the electronic polaron effect have a rather weak influence on the field dependence of.

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