Tunneling mechanism for the formation of negative ions near the electrode

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The zero-radius potential method is used to analytically solve the problem of the tunneling mechanism for the production of negative ions for particles which have a positive affinity to an electron and which move in an electric field near the electrode. An expression is derived for the probability of the formation of a negative ion.

Moving atoms with a positive electron affinity or positive ions near the negative electrode in a strong field can give rise to an effective tunneling mechanism for the formation of negative ions which account for the charge transfer and which can play an important role in the discharge in gases and liquids immediately before the breakdown and also in the emission from surfaces, such as cathode spots, which break down. The results of Ref. 1, in which the probabilities for the capture of electrons at the stationary impurity centers as they tunnel through the metal-insulator-metal or semiconductor-insulator-metal structures were calculated, cannot be used, however, to calculate the probability for the formation of negative ions near the surface. A steady-state analysis of the trapping of a tunneling electron at the level of an atom or ion is incorrect, since at the thermal velocity of the particle $\bar{v} \sim 10^{-3}$ a.u. ($\sim 10^5$ cm/s) and width of the potential barrier $l \sim 100$ Å the transit time is $\tau_n \sim 10^{-11}$ s. This time may be much shorter than the time it takes a steady wave function to be established, $\tau_s \sim \Gamma^{-1} \times 10^{-16}$ s and $\Gamma \sim \exp[-\sqrt{2U}l]$, where U is the barrier height. For $U \sim 2 \times 10^{-1}$ a.u. (5 eV), we find $\tau_s \sim 5 \times 10^{-3}$ s.

It is difficult to solve this problem with allowance for the change in the distance between the particle and the electrode and the change in the relative depth of the potential well corresponding to the level of the particle that moves in the field (Fig. 1). A change in the particle coordinate, however, does not appreciably affect, as will be shown below, the amplitude of the capture. We have therefore solved the problem of the capture of an electron with a fixed energy as a result of tunneling interaction with a stationary point potential well of variable depth. The problem was solved by using a well-known method of zero-radius potentials.[2] Let us consider an electron with a momentum $p_z = \sqrt{2E_0}$, which is tunneling through a barrier $W(r)$ which contains a center at the point $r = 0$ and which is characterized by an energy level $\epsilon = \epsilon(t)$. The general solution of the Schrödinger equation is

$$\psi(r,t) = \psi_0(r)\exp[-iE_0 t] + \int_\Gamma gG_E(r,0)\exp[-iEt]\,dE, \qquad (1)$$

where $G_E(r,0)$ is the Green's function of an electron in the potential $W(r)$, and Γ is

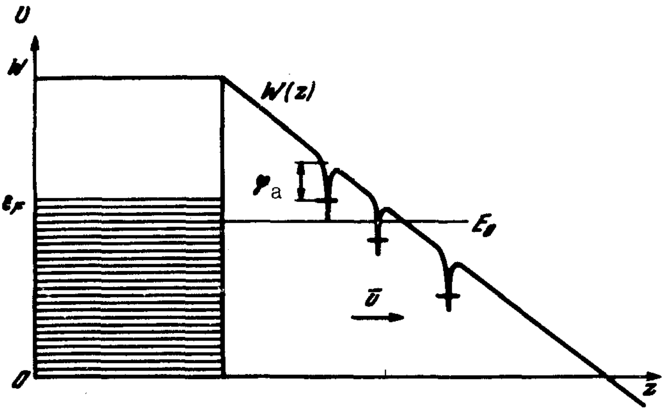

FIG. 1.

the contour in the complex E plane. In the limit $r \to 0$ the boundary condition is

$$\psi_{r\to 0} = C\left(\frac{1}{r} - \kappa(t)\right), \tag{2}$$

where $\kappa(t) = \sqrt{2\epsilon(t)}$. In the case of motion of an atom away from the electrode we have

$$\frac{d\kappa}{dt} = \frac{\epsilon'(t)}{\sqrt{2\epsilon(t)}} \sim \frac{\bar{v}f}{\sqrt{2(W_0 - E_0)}} \equiv \beta , \tag{3}$$

where f is the field strength. For $f \sim 10^{-3}$ a. u. $\bar{v} \sim 10^{-3}$ a.u. $[W(0) - E_0] \sim 10^{-1}$ a.u., and $\beta \sim 10^{-(5-6)}$. If $\kappa(t) = \beta t$, assuming

$$i\beta g \exp[-iEt]\,\Big|_{\Gamma_1}^{\Gamma_2} = \psi_0(r)\exp[-iE_0 t], \tag{4}$$

we find

$$g(E) = N\exp\Big[-\frac{i}{\beta}\int^{E} G^{p}_{E'}\,dE'\Big], \tag{5}$$

where N is a normalization factor, and $G^{p}_{E'}$ is the regular part of the Green's function. The contours Γ and N are determined from substitution (4) and from the requirement that the scattered wave attenuate in the limit $|t| \to \infty$. It is obvious that $\Gamma_1 = E_0$ and $|N| = |\psi_0/\beta|$. For a wide barrier, within terms of order $\exp[-\sqrt{2(W(0) - E)l}]$, we have $G^{p}_{r\to 0} \approx -\sqrt{2(W)(0) - E)l}$ and

$$g(E) = N\exp\Big[-\frac{i}{\beta}\,\frac{(2(W(0) - E))^{3/2}}{3}\Big]. \tag{6}$$

Transforming to the variable $u = \sqrt{2(W(0) - E)}$ and assuming $r \sim 0$, we find the following expression for a scattered wave:

$$\psi_p(r)_{r\sim 0} = -\frac{N\exp[-iW(0)t]}{r}\int_\Gamma \exp\left[-\frac{i}{3\beta}u^3 + \frac{i}{2}u^2 t\right]u\,du, \qquad (7)$$

where the contour Γ begins at the point $u_0 = \sqrt{2(W(0) - E_0)}$ and in the complex u plane goes to infinity in the region where the integral converges, and $\psi_p \to 0$ as $|t| \to \infty$. If $\beta > 0$ and $\beta t < u_0$, the integration path, which satisifies the indicated conditions, is illustrated in Fig. 2 {the dashed line and the hatching where $\mathrm{Re}[-(i/3\beta)u^3 + (i/2)u^2 t] > 0$}. If $\beta t > u_0$, the path can be drawn through the saddle point $u = \beta t$ (the solid line in Fig. 2). Evaluating the integral as a sum of contributions from the regions near u_0 and βt, we find the trapping probability (the contribution to the integral from the saddle point)

$$\omega' \sim \frac{\pi}{\beta}|\psi_0(0)|^2 . \qquad (8)$$

The trapping time is $\tau_3 \sim 1/\sqrt{\beta}$ a.u. ($\sim 10^{-13}$ s). Since the particle coordinate changes in a time $\tau_3 \sim 1$ Å (i.e., it is short), its disregard contributes only slightly to the error in estimating the trapping probability. The total probability for the formation of a negative ion can be estimated by summing over all metal electrons in the Sommerfeld model. In the simple case $T = 0$ an analytic estimate can be obtained for ω in atomic units:

$$\omega \sim \frac{n_0}{32\pi v W}\sqrt{\frac{\varphi_{\mathrm{cp}}}{\epsilon_F}}\exp\left[\frac{2}{3f}\{(2\varphi_{\mathrm{cp}})^{3/2} - (2W)^{3/2}\}\right], \qquad (9)$$

where φ_a is the energy of the affinity of the atom to an electron, W is the work

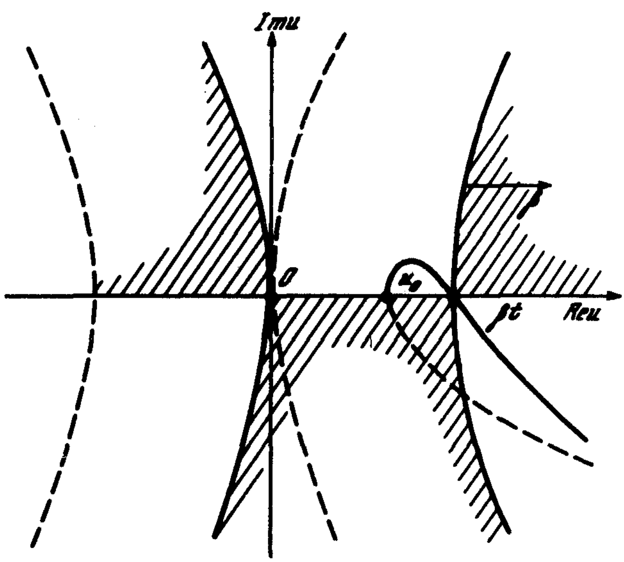

FIG. 2.

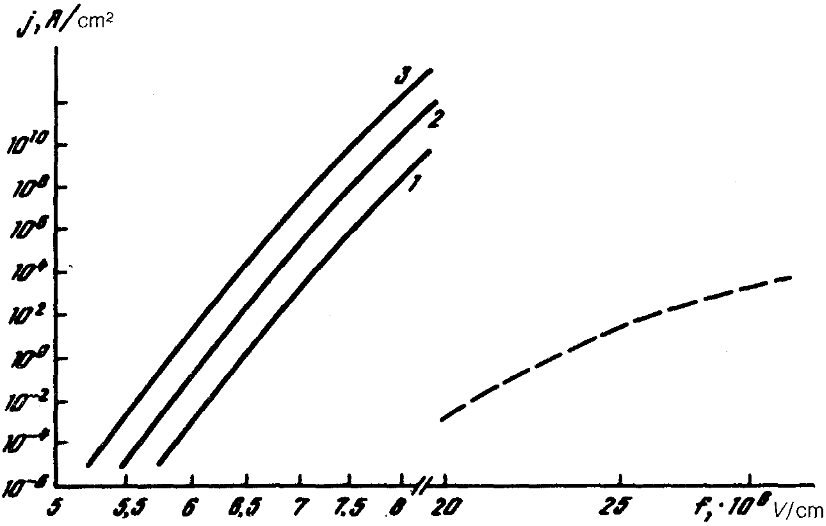

FIG. 3. Comparison of the current density due to the tunnel trapping of electrons at various gas concentrations with the current density of the Fowler-Nordheim field emission (dashed curve). 1–$N_a = 10^{17}$ cm^{-3}; 2–$N_a = 10^{19}$ cm^{-3}; 3–$N_a = 10^{21}$ cm^{-3}.

function of the electrode, n_0 is the atomic scale of the concentration, and $n_0 \approx 6.7 \times 10^{24}$ cm^{-3}. The current density due to the tunneling generation of negative ions in this case is $j \sim \omega \bar{v} N_a$, where N_a is the concentration of atoms in the interelectrode gap. The current density is plotted in Fig. 3 as a function of the field strength for various values of N_a for the system copper electrode-electrode gas. We see that even at low concentrations of the atoms the tunneling attachment of electrons manifests itself at relatively low field strengths close to those of the breakdown point. Shown for comparison is a plot of the Fowler-Nordheim field-emission current density.

The definitive expression for the tunnel current which is associated with the production of negative ions incorporates the volume concentration of atoms with a positive affinity to an electron, in contrast with that found in Ref. 1, where the principal contribution to the tunneling current comes from the atoms situated in a fairly narrow layer and where the magnitude of the tunneling current is porportional to the planar concentration of such atoms.

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[2]Yu. N. Demkov and V. N. Ostrovskiĭ, Zero-Radius Potential Method in Atomic Physics, State University, Leningrad, 1975.

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