

PROBABILITY OF ELECTRON TUNNELING THROUGH DIELECTRIC PORES IN SURFACE METAL LAYER

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The paper presents a study of the influence of nanovoids formed in the metal surface layer on the field emission current (the first stage of the accelerator structure breakdown). It is shown that the field emission current through nanovoids has a resonant character. It was found that under resonant conditions, an increase in the current density from the copper surface by more than 3.5 times compared to the case of an unmodified surface is observed. The presence of a dielectric in the nanovoids expands the resonant region. When the resonance conditions are not met or the diameter of the nanovoids increases, the current density decreases to zero, which can be a way to prevent an accelerator structure breakdown.

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INTRODUCTION

During the passage of a beam of charged particles, the walls of the accelerator are irradiated. One of the types of radiation defects formed during irradiation is pores. During the study of the structural materials of the future compact linear collider (CLIC), it was found that the surface layer of copper (the main material of the future collider) at a depth of about 0.5 μm is heavily damaged by pores. The authors of this work emphasize that the cause of such phenomena is the penetration of relatively insoluble gases (in particular, hydrogen) into the metal volume [1].

Paper [2] states that theoretical and modeling works at the University of Helsinki indicate that the presence of voids (several nm in diameter) near the cathode surface make a significant contribution to the vacuum breakdown mechanism.

Paper [3] deals with the formation of pores in the near-surface layer by diffusion of hydrogen ions. These “bubbles” with hydrogen can subsequently form irregularities on the surface. Similar results are presented in [4]. It states that despite the heat treatment of the electrodes, the measurements revealed that hydrogen from 2 to 5 ppm was present in copper samples. At the same time, the theoretical diffusion model states that no hydrogen should remain after heat treatment. Its presence indicates that such extensive heat treatment increases the number of vacancies filled with hydrogen.

Papers [5, 6] consider issues related to the formation of blisters – bubbles on the metal surface. Their formation is a common effect on the surface of a metal exposed to irradiation. This harmful effect was observed in Al, Fe, SS, and under certain conditions in Nb. And more importantly, it penetrates Cu, which is the first candidate for high-energy accelerating structure’s materials. The authors emphasize that hydrogen tends to penetrate copper and accumulate in some voids near the surface. In the modeling, the authors show atomistic mechanisms of bubble and blister growth under hydrostatic internal hydrogen pressure. All this leads to the conclusion that dielectric, in particular hydrogen, can accumulate in the near-surface layer. Therefore, the study of the effect of dielectric inclusions in the metal

surface layer is important and requires further investigation.

The Institute of Applied Physics of the National Academy of Sciences of Ukraine has for a long time been studying the mechanisms of high-voltage, high-vacuum breakdowns in the accelerating structures of modern ion/electron accelerators and the possibility of reducing the probability of their occurrence in order to increase their electrical stability.

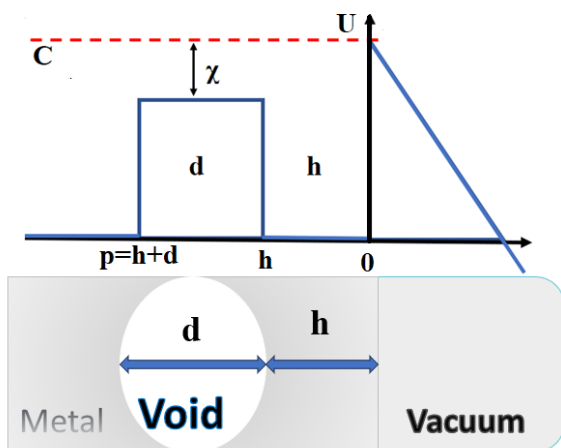
Thus, the influence of an external magnetic field [6–10] and relativistic effects [11, 12] on the field emission current was investigated. Papers [13–15] are devoted to the study of the presence of nanoscale irregularities in the near-surface region of a metal. And in [16], the process of heating and melting of such irregularities was investigated. At the same time, a large part of the work performed at the IAP NASU was devoted to the study of the effect of hydrogen on plasma formation during high-vacuum, high-gradient breakdown [17–26]. Based on the experimental data obtained at the DC-spark system (CERN) for measuring the optical spectrum of plasma clusters after high-voltage breakdown, it was first established that high-intensity optical hydrogen lines were present in the optical spectrum of a high-purity copper sample. In 2011, the ERDA channel of the IAP NASU accelerator began measuring the concentration of plasma hydrogen under conditions of a high concentration gradient in high-purity copper samples [21, 22]. Studies conducted at CERN by optical spectroscopy of the sample showed the presence of hydrogen in the sample spectrum [25].

In this paper, we theoretically study the effect of nano-sized pores filled with a dielectric, in particular hydrogen, on the field emission current from accelerator constriction materials as the first stage of the high-vacuum high-gradient breakdown.

1. CALCULATION OF THE FEE CURRENT FROM A MODIFIED SURFACE

To consider the presence of voids in the metal surface, we chose a double potential barrier model (Fig. 1). Such a barrier is considered to estimate the value of the field emission current from cathodes consisting of thin layers of non-homogeneous conductive materials [27,

In the case of the presence of a dielectric in the near-surface metal layer, the height of the rectangular step decreases by the value of the electron affinity energy χ .


$$j = \int_0^{\mu} N(W)D(W)dW, \quad (1)$$

To calculate the probability of electron tunneling through the barrier, the one-dimensional time-independent Schrödinger equation is solved,

$$-\frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + [U(x) - W] \psi(x) = 0, \quad (2)$$

where $\psi(x)$ is complex wave function of the electron, $\hbar$ is Planck's reduced constant, m is a mass of an electron, $U(x)$ is a potential and W is initial longitudinal energy of electrons falling on the metal surface. For simplicity, the mass of the electron m in all three regions (i.e., in the metal, dielectric, and vacuum) is assumed to be equal to the rest mass of the electron.

$$\begin{aligned}\psi_1 &= e^{ik\sqrt{W}x} + B_1 e^{-ik\sqrt{W}x}, \\ \psi_2 &= A_2 e^{k\sqrt{V}x} + B_2 e^{-k\sqrt{V}x}, \\ \psi_3 &= A_3 e^{ik\sqrt{W}x} + B_3 e^{-ik\sqrt{W}x}, \\ \psi_4 &= T(Ai(-\eta) - iBi(-\eta)),\end{aligned}\tag{3}$$

The transmission coefficient of a potential barrier is defined as the ratio of the probability of current density that has passed to the probability of current density of the flow:

$$D(W) = \frac{I_{trans}(W)}{I_{inc}(W)}. \quad (4)$$

$$J = \frac{i\hbar}{2m(\psi\nabla\psi^* - \psi^*\nabla\psi)}. \quad (5)$$
$$\begin{aligned}\psi_{inc} &= e^{ik\sqrt{W}x}, \\ \psi_{trans} &= T(Ai(-\eta) - iBi(-\eta)).\end{aligned}\quad (6)$$
$$\begin{aligned} j_{inc} &= k\sqrt{W}, \\ j_{trans} &= \frac{\xi}{\pi}|T^2|. \end{aligned} \quad (7)$$
$$D(W) = \frac{\xi}{\pi k \sqrt{W}} |T^2|. \quad (8)$$
$$\begin{cases} \frac{\partial \psi_1}{\partial x} = ik\sqrt{W}e^{ik\sqrt{W}x} - ik\sqrt{W}B_1e^{-ik\sqrt{W}x} \\ \frac{\partial \psi_2}{\partial x} = k\sqrt{V}A_2e^{k\sqrt{V}x} - k\sqrt{V}B_2e^{-k\sqrt{V}x} \\ \frac{\partial \psi_3}{\partial x} = ik\sqrt{W}A_3e^{ik\sqrt{W}x} - ik\sqrt{W}B_3e^{-ik\sqrt{W}x} \\ \frac{\partial \psi_4}{\partial x} = T(-\xi Ai'(-\eta) + i\xi Bi'(-\eta)). \end{cases} \quad (9)$$
$$D = \frac{4(C - \chi - W)W^{\frac{3}{2}}e^{-\frac{4k(C-W)^{\frac{3}{2}}}{3eE}}\sqrt{C-W}}{(C-\chi)(L+WR^2) - W^2C}, \quad (10)$$

$$\begin{aligned} \text{where } Y &= \sqrt{C-W} \sin(\alpha h) + \cos(\alpha h) \sqrt{W}, \\ L &= (\sinh(\beta d) Y \sqrt{C-\chi-W} + \cosh(\beta d) \sqrt{W} \Lambda)^2, \\ \Lambda &= \sqrt{C-W} \cos(\alpha h) - \sin(\alpha h) \sqrt{W}, \alpha = k\sqrt{W}. \end{aligned}$$

$$\beta = k\sqrt{C - \chi - W}, k = \frac{\sqrt{2m}}{h}, V = C - W - \chi, \\ \eta = \xi \left(x - \frac{C-W}{eE} \right).$$

In case of $h = d = 0, \chi = 0$ this equation is transformed into the Fowler-Nordheim equation [28], which confirms the fulfillment of the correspondence principle.

$$D = \frac{4\sqrt{W} e^{-\frac{4k(C-W)^{\frac{3}{2}}}{3eE}} \sqrt{C-W}}{C}. \quad (11)$$

From equation (10), it can be seen that the field emission current from a metal-dielectric-metal-vacuum system strongly depends on the thickness of the dielectric layer. As the thickness of the effective layer d increases, the current will decrease exponentially. At the same time, the dependence on the depth of the dielectric layer is in the form of a sine and cosine argument. This means that the current must be oscillatory. It is easy to see that the maximum condition will be:

$$h = \frac{\pi}{2\alpha}(2n+1), n = 0, 1, 2, \dots \quad (12)$$

2. FIELD EMISSION CONSIDERING PORES FILLED WITH DIELECTRIC

Another important question is how the current density of field electron emission from accelerator construction materials will change in the case of filling the pores with a dielectric, i.e., from the metal-dielectric-metal-vacuum system. Table shows the values of the affinity energy per atom for some gases that can penetrate the pores in the metal surface layer [30].

№	Element	Name	Electron affinity, eV/atom
1	^1H	Hydrogen	0.754
2	^2H	Deuterium	0.755
3	C	Carbon	1.262
4	O	Oxygen	1.461
5	O ₂	Dioxygen	0.45

Upon further consideration, we chose different values of the electron affinity energy in the range of $\chi = 0 - 2$ eV. This is since only a few atoms can be located in voids of this size at the one time. And based on Table, the affinity energy will take values within these limits.

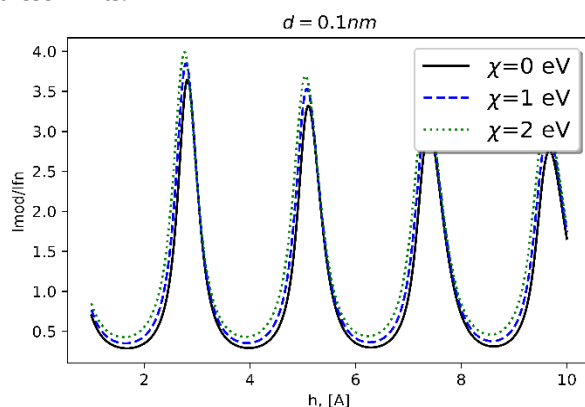


Fig. 2. Comparison of the field emission current densities j_{mod} and j_{F-N} depending on χ and h for $h=0 \dots 1$ nm

It was shown in [13] that for the parameters of accelerator structures, the influence of a generalized layer of pores with a diameter of 0.1 nm will be most noticeable. Therefore, to study the effect of pore filling with a dielectric, we chose an effective layer of this thickness to ensure the best visibility of the results. Fig. 2 shows the dependence of the field emission current, expressed in units of Fowler-Nordheim current, on the depth of the defect for different affinity energies χ .

Fig. 2 shows that the current character in the case of filling the pores with a dielectric with different affinity energies remains the same. The current also has a resonant character. In the region of resonant amplification, the field emission current density increases by about 3.5 times for a given set of affinity energies. It is worth noting that the current enhancement associated with a decrease in the step height at the potential barrier (see Fig 1) due to the electron affinity does not exceed 10%. From Fig. 2, it can be concluded that with an increase in the depth h , the character of the emitted current retains an oscillatory character with a weak damping.

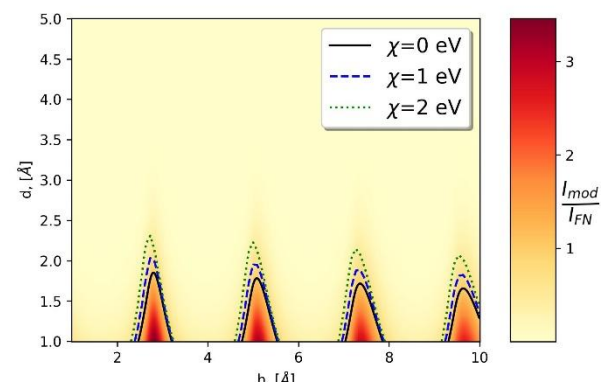


Fig. 3. Color map of the current density from the modified surface j_{mod} , expressed in units of current from an ideal surface j_{F-N} for different void sizes d and metal layer thickness h in the case $\chi = 0$. The contour line is the value of $j_{mod}/j_{F-N} = 1$ for different electron

affinity energies

To find the effect of both the thickness of the effective layer d and the depth h on the field emission current, we plotted a color map of the current from the modified metal surface (Fig. 3). It shows the results of the numerical calculation of the field emission current density when $\chi = 0$ expressed in units of current from an ideal surface. The contour lines show the areas where the current from the modified surface is higher than the current from the unmodified surface for different electron affinity energies $\chi = 0, 1, 2$ eV.

The Fig. 3 shows that the current is indeed resonant. It is also worth noting that in the case when the thickness of the effective layer is $d > 0.25$ nm a decrease in the field electron emission current will be observed, regardless of the depth of their occurrence. An increase in the affinity energy contributes to an increase in the resonance region in the d and h coordinates. At the same time, based on the small size of d , which leads to an increase in current, it can be concluded that the pres-

ence of micron and submicron defects in the metal surface layer can reduce the field emission current density and increase the breakdown resistance of the structure. The presence of a dielectric in such voids enhances the resonance effect.

SUMMARY

The influence of submicron defects in the metal surface layer on the field emission current as the main factor of breakdown occurrence is theoretically investigated. The analysis of literature has shown that the presence of nanoscale voids filled with hydrogen can be a factor influencing the breakdown.

Studies have shown that the electron emission current near nanovoids on a metal surface shows an oscillatory resonant character that depends on the depth of the nanovoid h . In the case of fulfillment of the resonance conditions (12), the current density of field electron emission from the modified copper surface is higher than the current density from the unmodified surface by more than 3.5 times. An increase in the size of the nanovoid (or effective layer d) leads to a rapid decrease of the field emission current.

The presence of a dielectric in the voids widens the resonant region. The increase is about 10% for $\chi = 1$ eV and about 20% for $\chi = 2$ eV. If the resonance conditions are not met or if the diameter of the nanopores is increased, the current density drops sharply, close to zero, which can be a way to prevent breakdown.

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APPENDIX

Given that at the metal-dielectric interface $x = -p$, at the dielectric-metal interface $x = -h$ and at the metal-vacuum interface $x = 0$ we obtain the following system of equations:

$$\begin{cases} e^{-ik\sqrt{W}p} + B_1 e^{ik\sqrt{W}p} = A_2 e^{-k\sqrt{V}p} + B_2 e^{k\sqrt{V}p} \\ ik\sqrt{W}e^{-ik\sqrt{W}p} - ik\sqrt{W}B_1 e^{ik\sqrt{W}p} = k\sqrt{V}A_2 e^{-k\sqrt{V}p} - k\sqrt{V}B_2 e^{k\sqrt{V}p} \\ A_2 e^{-k\sqrt{V}h} + B_2 e^{k\sqrt{V}h} = A_3 e^{-ik\sqrt{W}h} + B_3 e^{ik\sqrt{W}h} \\ k\sqrt{V}A_2 e^{-k\sqrt{V}h} - k\sqrt{V}B_2 e^{k\sqrt{V}h} = ik\sqrt{W}A_3 e^{-ik\sqrt{W}h} - ik\sqrt{W}B_3 e^{ik\sqrt{W}h} \\ A_3 + B_3 = T(Ai(y) - iBi(y)) \\ ik\sqrt{W}A_3 - ik\sqrt{W}B_3 = T(-\xi Ai'(y) + i\xi Bi'(y)), \end{cases}$$

where $y = \xi \frac{C-W}{eE}$. By solving the system of equations, we find T : $T = \frac{8ikW\sqrt{V}e^{-ik\sqrt{W}p}}{Real + i Imag}$. Where the following notations are introduced: $Real = 4 \sinh(k\sqrt{V}d) \left((AiryAi(y) \cos(k\sqrt{W}h) k\sqrt{W} + \xi AiryAi(1, y) \sin(k\sqrt{W}h))V + \right.$

$AiryBi(y) \sin(k\sqrt{W}h) kW^{\frac{3}{2}} - \xi AiryBi(1, y) \cos(k\sqrt{W}h) W \Big) + 4\sqrt{V} \cosh(k\sqrt{V}d) \left((AiryBi(y) \cos(k\sqrt{W}h) + \right.$
 $AiryAi(y) \sin(k\sqrt{W}h))kW - (AiryAi(1, y) \cos(k\sqrt{W}h) - AiryBi(1, y) \sin(k\sqrt{W}h))\xi\sqrt{W} \Big), Imag =$
 $-4 \sinh(k\sqrt{V}d) \left((AiryAi(y) \sin(k\sqrt{W}h) kW^{\frac{3}{2}} - \xi W AiryAi(1, y) \cos(k\sqrt{W}h) - (AiryBi(y) \cos(k\sqrt{W}h) k\sqrt{W} + \right.$
 $\xi AiryBi(1, y) \sin(k\sqrt{W}h))V \Big) + 4\sqrt{V} \cosh(k\sqrt{V}d) \left(kW(AiryAi(y) \cos(k\sqrt{W}h) - AiryBi(y) \sin(k\sqrt{W}h)) + \right.$
 $\xi\sqrt{W} (AiryAi(1, y) \sin(k\sqrt{W}h) + AiryBi(1, y) \cos(k\sqrt{W}h)) \Big)$. Then the square of the modulus of the amplitude of the transmitted wave $|T^2|$ can be written in the form: $|T^2| = \frac{64k^2W^2V}{Real^2 + Imag^2}$.

Using formula (8), we write the transmission coefficient of the potential barrier: $D = \frac{64\xi V kW^{\frac{3}{2}}}{\pi(L+Y)}$,

where the following symbols are introduced:

$$L = \left(-4 \sinh(k\sqrt{V}d) \left(\text{Ai}(y) \sin(k\sqrt{W}h) kW^{\frac{3}{2}} - \xi W \text{Ai}'(y) \cos(k\sqrt{W}h) - (\text{Bi}(y) \cos(k\sqrt{W}h) k\sqrt{W} + \xi \text{Bi}'(y) \sin(k\sqrt{W}h))V \right) + 4\sqrt{V} \cosh(k\sqrt{V}d) \left(kW(\text{Ai}(y) \cos(k\sqrt{W}h) - \text{Bi}(y) \sin(k\sqrt{W}h)) + \xi\sqrt{W}(\text{Ai}'(y) \sin(k\sqrt{W}h) + \text{Bi}'(y) \cos(k\sqrt{W}h)) \right) \right)^2 Y = \left(-4 \left((\text{Ai}(y) \cos(k\sqrt{W}h) k\sqrt{W} + \xi \text{Ai}'(y) \sin(k\sqrt{W}h))V + \text{Bi}(y) \sin(k\sqrt{W}h) kW^{\frac{3}{2}} - \xi \text{Bi}'(y) \cos(k\sqrt{W}h) W \right) \sinh(k\sqrt{V}d) + 4 \left((\text{Bi}(y) \cos(k\sqrt{W}h) + \text{Ai}(y) \sin(k\sqrt{W}h))kW - (\text{Ai}'(y) \cos(k\sqrt{W}h) - \text{Bi}'(y) \sin(k\sqrt{W}h))\xi\sqrt{W} \right) \cosh(k\sqrt{V}d) \sqrt{V} \right)^2.$$

For the parameters at which field electron emission from the structural materials of accelerator structures usually takes place, namely, copper material and an electric field of $E = 100 \frac{MV}{m}$ the parameter y takes large values ($y=68.94$), so it is possible to estimate the values of special Airy functions using their asymptotic approximation [31, 32]:

$$\text{Ai}(y) = \frac{e^{-\frac{2y^{\frac{3}{2}}}{3}}}{2\sqrt{\pi}y^{\frac{1}{4}}}, \text{Bi}(y) = \frac{e^{\frac{2y^{\frac{3}{2}}}{3}}}{y^{\frac{1}{4}}\sqrt{\pi}}, \text{Ai}'(y) = -\frac{e^{-\frac{2y^{\frac{3}{2}}}{3}}}{2\sqrt{\pi}} \frac{1}{y^{\frac{5}{4}}}, \text{Bi}'(y) = \frac{y^{\frac{1}{4}}e^{\frac{2y^{\frac{3}{2}}}{3}}}{\sqrt{\pi}}.$$

It is easy to see that only functions with a positive exponent will play a significant role. Therefore, the terms $\text{Ai}(y)$ and $\text{Ai}'(y)$ can be neglected for the given parameters of the problem. Then the transparency coefficient of the

potential barrier D will take the form: $D = \frac{4\xi V kW^{\frac{3}{2}}}{\pi(L_1 + Y_1)}$,

where the following symbols are introduced:

$$L_1 = \left(\sinh(k\sqrt{V}d) \left((\text{Bi}(y) \cos(k\sqrt{W}h) k\sqrt{W} + \xi \text{Bi}'(y) \sin(k\sqrt{W}h))V \right) - \sqrt{V} \cosh(k\sqrt{V}d) \left(kW(\text{Bi}(y) \sin(k\sqrt{W}h)) - \xi\sqrt{W}(\text{Bi}'(y) \cos(k\sqrt{W}h)) \right) \right)^2, \\ Y_1 = \left(- \left(\text{Bi}(y) \sin(k\sqrt{W}h) kW^{\frac{3}{2}} - \xi \text{Bi}'(y) \cos(k\sqrt{W}h) W \right) \sinh(k\sqrt{V}d) + \left((\text{Bi}(y) \cos(k\sqrt{W}h))kW + (\text{Bi}'(y) \sin(k\sqrt{W}h))\xi\sqrt{W} \right) \cosh(k\sqrt{V}d) \sqrt{V} \right)^2.$$

When calculating the field emission from the structural materials of accelerators, asymptotic approximations for the Airy functions $\text{Bi}(y)$ and $\text{Bi}'(y)$ presented above can be used.

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ЙМОВІРНІСТЬ ТУНЕЛЮВАННЯ ЕЛЕКТРОНІВ ЧЕРЕЗ ДІЕЛЕКТРИЧНІ ПОРИ У ПОВЕРХНЕВОМУ ШАРІ МЕТАЛУ

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Представлено дослідження впливу нанопор, сформованих у поверхневому шарі металу, на струм польової емісії (перший етап виникнення пробою прискорювальної структури). Показано, що струм польової емісії через нанопори має резонансний характер. Виявлено, що в резонансних умовах спостерігається збільшення густини струму з поверхні міді більш ніж у 3,5 рази порівняно з випадком немодифікованої поверхні. Наявність діелектрика у нанопорах розширює резонансну область. Коли умови резонансу не виконуються або діаметр нанопор збільшується, густина струму зменшується до нуля, що може бути способом запобігання пробою.