

# DETERMINATION OF THE SPECTRA OF ION He AND H<sub>2</sub> BOMBARDMENT OF AUTOEMITTER SURFACE

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Analytical consideration and numerical calculations of the parameters describing the operating conditions of field electron emitters and the spectra of the ion bombardment of emitting surface are adduced. Based on the analysis of the obtained energy spectra, it is calculated the dependence of the average energy of bombarding ions of helium and hydrogen on the radius of curvature of the emitter in the process of field current extraction and it is proposed an analytical approximation of the results.

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## INTRODUCTION

The development of radiation-resistant materials of reactor building largely complicated by the lack of knowledge of the nature of radiation effects in the relatively unexplored region of very high doses. In works [1, 2] using accelerator simulation technologies there were investigated in detail the processes of interaction of fast charged particles with solids: primary radiation damage of materials, formation and evolution of dislocation structure. As the result, it was achieved a significant progress in the development of concepts of radiation damage of structural materials. However, there are still insufficiently studied experimentally the phenomena accompanying the elementary acts of radiation damage. In this regard, of particular interest are simulated experiments in situ using field ion microscopes with built-in sources of accelerated ions [3, 4]. In such experiments at the atomic level there were detected processes such as surface diffusion, activated by low-energy ion bombardment [5, 6], which play an essential role in radiation damage of materials of the first wall and divertor of fusion devices and is widely used at present in nanotechnology of surface treatment of metals.

For irradiation of solids by low-energy ions in the chamber of field emission microscope was used method [7, 8], based on the bombardment of the surface of the needle-shaped sample by ions formed by electron impact ionization of atoms (molecules) of gas that fills the vacuum chamber of the microscope. The resulting ions are accelerated in a strong electric field and bombard the surface of the needle-shaped sample. This technique allows varying in a wide interval of ion beams parameters up to the minimum, corresponding to a single ion collision with the surface, allowing the study of elementary acts of radiation damage. Since using this method there is no possibility of direct experimental determination of the intensity of the ion bombardment of the sample surface, it is necessary to conduct their numerical calculations. Recently in a number of works [9, 10], there was established an analytical framework for calculations of ion bombardment of needle samples in the process of field current extraction. However, these calculations was not took into account found in the work of P.A. Bereznyak and V.V. Slezov [8] features of the configuration space region from which ions, generated with zero initial

speed, get to the emitting part of the sample. The present article shows the results of calculations of the ion bombardment of the needle samples in the process of field current extraction that are performed in the framework of Bereznyak-Slezov theory for a wide range of irradiation parameters.

## RESULTS AND DISCUSSION

### 1. SIMULATION OF ION SPECTRA

The potential distribution near the surface of the needle emitter and in the interelectrode space is satisfactorily described by Bereznyak-Slezov model [8], originally developed to solve the problem of ion bombardment of needle-shaped emitters. The authors convincingly showed that the most part of the ions, formed in the process of field current extraction, bombards the side (tapered) part of the emitter. Emitting region is bombarded mainly from the axial cylindrical region of radius  $4.8r_0$ . However, it should be noted that due to the large amount of calculations and the limited memory and speed of used computers, the task was strictly solved only for one set of parameters specific to the field emitters.

In this work, we present the results of the analysis and the numerical values of the relevant parameters describing the operating conditions of field electron emitters and the spectra of the ion bombardment of emitting surface. The calculations were performed using Bereznyak-Slezov approximation. The equations of motion of a particle with charge  $e$  and mass  $m$ , according to this model are of the form:

$$\ddot{\eta} = \frac{e}{mr_0} \left( -\frac{1}{r_0} \cdot \frac{\partial \varphi}{\partial \eta} \right); \quad \ddot{\gamma} = \frac{e}{mr_0} \left( -\frac{1}{r_0} \cdot \frac{\partial \varphi}{\partial \gamma} \right); \quad (1)$$

$$\ddot{\eta} = -\frac{e}{mr_0^2} \frac{V}{C_K - C_A} \left[ \varpi \eta (\gamma^2 + \eta^2)^{-3/2} + (\gamma^2 + \eta^2)^{-1/2} \right]; \quad (2)$$

$$\ddot{\gamma} = -\frac{e}{mr_0^2} \frac{V}{C_K - C_A} \left[ \varpi \gamma (\gamma^2 + \eta^2)^{-3/2} + \frac{\gamma (\gamma^2 + \eta^2)^{-1/2}}{\sqrt{\gamma^2 + \eta^2 + \eta}} \right]. \quad (3)$$

$\ddot{\eta}$  and  $\ddot{\gamma}$  are interpreted as the components of acceleration along the axis and perpendicular to the axis, respectively. Solving this system in the time scale  $\tau$ , it can be set polar coordinate of the point of ion contact on the edge. Here

$$1\tau = r_0 \sqrt{\frac{m}{|e|} \cdot \frac{C_K - C_A}{V}}. \quad (4)$$

For determination of the intensity of ion bombardment, we used the approximation formula for the configuration area, from which ions, formed with zero initial velocity, fall on the needle top:

$$\gamma_0(\eta) = \gamma_m + \frac{A_1 - \gamma_m}{1 + \exp((\eta - \eta_0)/\Delta\eta)}, \quad (5)$$

where  $\gamma_m = 4.80368$ ;  $A_1 = -2485.07$ ;  $\eta_0 = -18.6127$  and  $\Delta\eta = 2.7592$ .

From (5) it follows that the contribution to ion bombardment of emitting surface is provided by the ions formed near the surface of the tip, or in a region close to the symmetry axis. In both cases, for the number of ions  $N$ , bombarding the surface per time unit the ratio is applicable:

$$N(\eta) = \frac{p}{kT} \frac{j_0}{e} 2\pi r_0^3 \int_0^{\eta_{\max}} \int_{\gamma_{\min}(\eta)}^{\gamma_{\max}(\eta)} \frac{\gamma \sigma(\gamma, \eta)}{\gamma^2 + \eta^2} d\eta d\gamma, \quad (6)$$

$$N = k_{BS} \frac{p}{kT} \frac{I}{e} r_0 \sigma(V_0), \quad \eta \gg 10. \quad (7)$$

Here  $p$  is the pressure in the chamber of the microscope, Pa;  $k = 1.3806488 \cdot 10^{-23}$  – the Boltzmann constant, J/K;  $T$  – temperature, K;  $I$  – field current, A;  $e = 1.602176 \cdot 10^{-19}$  – the electron charge, C;  $\sigma(V_0)$  – the ionization cross section,  $m^2$ ;  $k_{BS}$  – Bereznyak-Slezov factor, is equal to:

$$k_{BS} = \int_{\eta_{\min}}^{1000\gamma_0(\eta)} \int_0^{\gamma_{\max}(\eta)} \frac{\Sigma(\eta) \cdot \gamma}{\eta^2 + \gamma^2} d\gamma d\eta, \quad (8)$$

where

$$\Sigma(\eta) = \frac{\frac{V(\eta)}{E_i} - 1}{\left(\frac{V(\eta)}{E_i}\right)^2} \ln\left(1.25 \cdot \frac{V(\eta)}{E_i}\right) \frac{\left(\frac{V_0}{E_i}\right)^2}{\left(\frac{V_0}{E_i} - 1\right) \cdot \ln\left(1.25 \cdot \frac{V_0}{E_i}\right)}. \quad (9)$$

Here  $\Sigma(\eta)$  is reduced ionization cross section;  $V(\eta)$  – the potential at a given point of the area;  $E_i$  – the ionization potential of the gas;  $\eta_{\min}$  – the distance where  $V(\eta_{\min}) = E_i$ .

Fig. 1 shows the dependence of the numerical coefficient  $k_{BS}$  determining the total number of ions bombarding the tip per time unit on the radius of curvature of the shape at the top for helium and hydrogen. Dots represent calculated values, and the solid curve is the proposed approximation:

$$\text{for hydrogen } k_{BS}(r_0)^H = 15.6 - 14.5 \cdot 0.9618^{r_0}, \quad (10a)$$

$$\text{for helium } k_{BS}(r_0)^{He} = 13.6 - 14.46 \cdot 0.9664^{r_0}. \quad (10b)$$

In numerical calculations, the operating voltage of the microscope (diode) was determined based on the condition of constancy of the field strength at the top of the emitter ( $F = 5$  V/nm). As follows from the Fig. 1, the coefficient  $k_{BS}$  significantly depends on the size of the emitter. The maximum value  $k_{BS}$  is 13.5 that is

consistent with calculations [8] carried out for the tip with a radius equal to 100 nm.

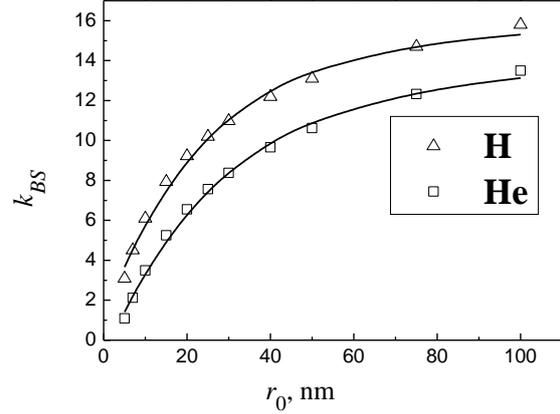


Fig. 1. The intensity of the ion bombardment of the tip depending on the radius of curvature of the emitter

From Fig. 2 it follows that the dependence of reduced ionization cross section of helium and hydrogen  $\Sigma(\eta)$  from the dimensionless axial coordinates (cylindrical system) has a sharp maximum near the shape top ( $r_0 = 100$  nm). For large values of coordinates and until the anode a cross section changes slightly.

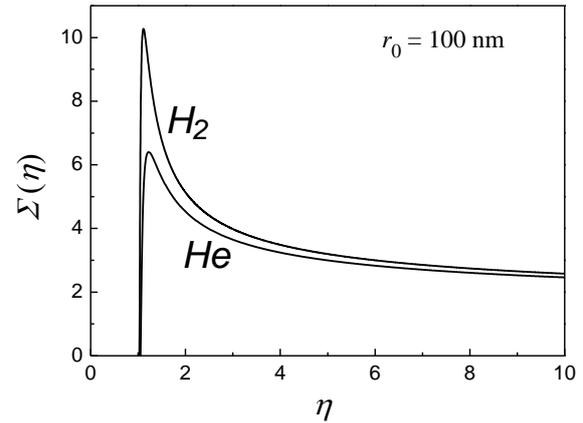


Fig. 2. Reduced ionization cross section of helium and hydrogen depending on the dimensionless coordinate directed along the optical axis

The distribution function for the energy of bombarding ions can be obtained from expressions (7) and (9):

$$f = \int_0^{\gamma_0(\eta)} \frac{\Sigma(\eta) \cdot \gamma}{\eta^2 + \gamma^2} d\gamma \cdot \left[ \frac{(2\eta_{\max} - 1)^{\frac{V(\eta)}{V_0}}}{2V_0} \cdot \ln(2\eta_{\max} - 1) \right]. \quad (11)$$

We have performed calculations for emitters with different radii of curvature at the top, corresponding to the typical conditions of the ion microscopy experiments. As the result, the curves of the energy distribution of bombarding ions were built.

Fig. 3 shows the energy spectra of ions of helium and hydrogen, bombarding the hemispherical part of emitters with radii of curvature of 10, 25, 50 and 100 nm, respectively. These values of the radii of curvature are typical for experiments with nanoemitters, samples, used in the traditional field ion microscopy, studying of the mechanisms of radiation damage of the

surface and operating of the needle nonheated cathodes in high-resolution electron microscopy.

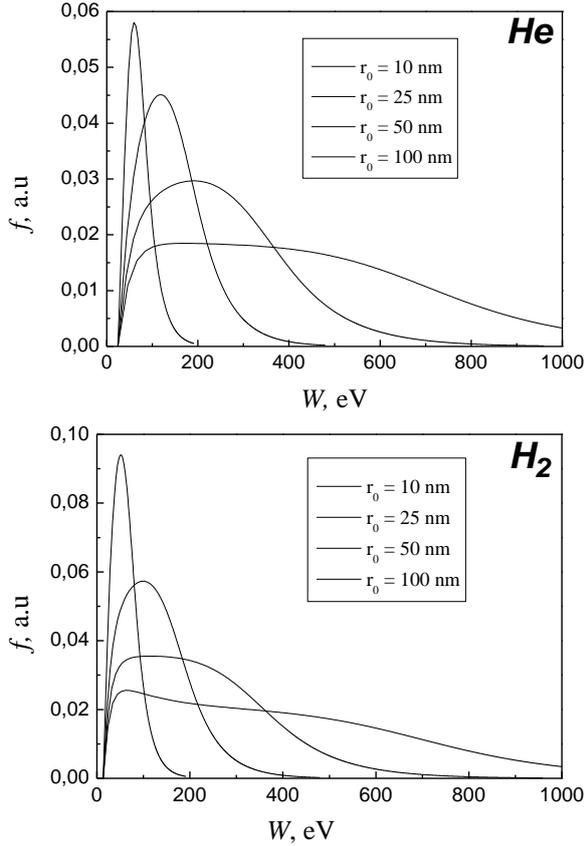


Fig. 3. Spectra of ion bombardment of the emitting part of the needle-shaped cathode with different radii of curvature in the process of field current extraction at the atmosphere of helium and hydrogen

## 2. CALCULATION OF THE ION BOMBARDMENT FLUENCE

Fig. 4 shows the dependence of the average energy of ion bombardment on the radius of curvature of the emitter in the process of field current extraction in the atmosphere of helium and hydrogen. The solid curve corresponds to calculations by the formula (11) obtained by numerical solution of the trajectory tasks. The dotted curve is the result of calculations by the approximate formula proposed in [5]. A comparison of these data shows an almost identical near the radii of curvature of the order of 50 nm, i.e., the area where the most ion-microscopic studies of radiation damage of autocathodes are carried out. Outside these values, there is only a slight deviation from the linear dependence, proposed on the basis of analytical calculations in [5].

To calculate the number of ions  $N$ , bombarding the surface of the tip per time unit (7) it is necessary to calculate the ionization cross section  $\sigma(W)$  of helium and hydrogen atoms. We used experimental data values  $\sigma(W)$  from [11, 12], and approximated them by formula:

$$\sigma(W) = A_1 \cdot \frac{W - A_2}{A_2 \cdot W^2} \cdot \ln \left( A_3 \cdot \frac{W}{A_2} \right). \quad (12)$$

where  $A_1 = 8317 \cdot 10^{-21}$ ;  $A_2 = 24.6$ ;  $A_3 = 0.986$  for helium and  $A_1 = 7130 \cdot 10^{-21}$ ;  $A_2 = 13.595$ ;  $A_3 = 0.92136$  for hydrogen.

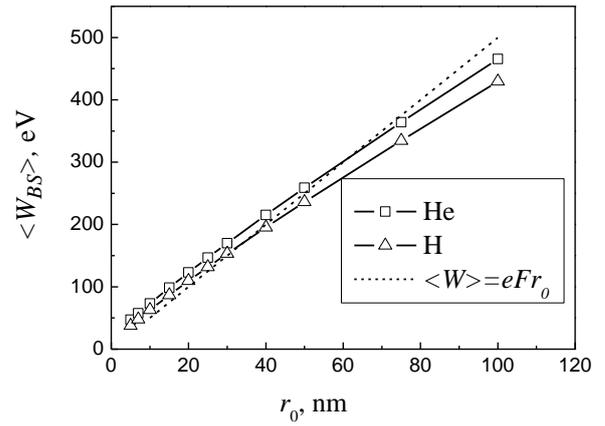


Fig. 4. The dependence of the average energy of ion bombardment on the radius of curvature of the emitter

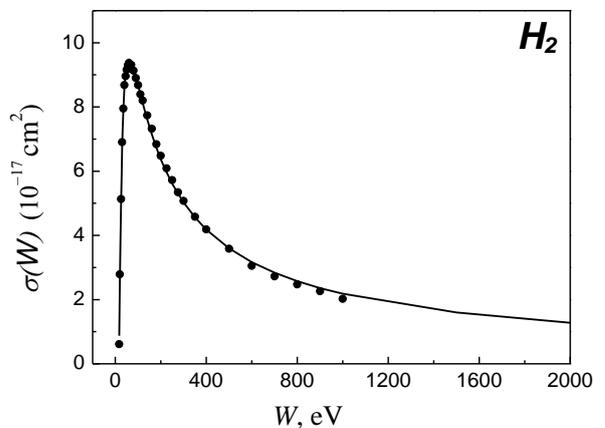
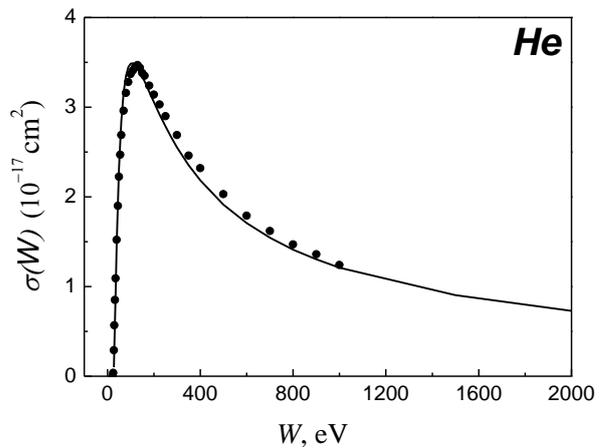


Fig. 5. The dependence of the ionization cross section on the electrons energy for helium and hydrogen

Fig. 5 shows the dependence of the ionization energy cross section on electrons energy for helium and hydrogen. Dots represent experimental data [11, 12], and the solid curve is the approximation formula (12).

Solving equation (7) considering (10a), (10b), (12) in terms of  $p = 0.01333$  Pa;  $T = 300$  K;  $I = 10^{-7}$  A;  $r_0 = 30$  nm;  $V_0 = 2$  kV, we obtain that each surface atom is subjected to a collision once on time of 152 c by helium ions and once on time of 66 c by hydrogen ions (assuming that  $1 \text{ cm}^2$  of the tip surface area contains  $10^{15}$  atoms). Hence the fluence of ions:

$$\Phi = \frac{N}{2\pi r_0^2} \cdot t \quad (13)$$

for time  $t = 100$  c is  $\Phi_{He} = 6.575 \cdot 10^{18} \text{ m}^{-2}$  for helium and  $\Phi_H = 15.14 \cdot 10^{18} \text{ m}^{-2}$  for hydrogen.

## CONCLUSIONS

A mathematical analysis and numerical calculations of the parameters describing the operating conditions of field electron emitters was performed and the spectra of the ion bombardment of emitting surface were obtained. There was established that at typical field emission researches of experimental conditions ( $F \leq 5 \text{ V/nm}$ ,  $r_0 \leq 100 \text{ nm}$ ) ions, formed when  $r \leq 10r_0$ , have energy below the threshold of radiation displacement of lattice atoms. There was established the dependence of the numerical coefficient  $k_{BS}$  determining the total number of ions bombarding the tip per time unit from the radius of curvature of the tip at the top. Based on the analysis of obtained energy spectra there was calculated dependence of the average energy of bombarding ions on the radius of curvature of the emitter in the process of field current extraction and analytical approximation results were proposed.

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## ОПРЕДЕЛЕНИЕ СПЕКТРОВ БОМБАРДИРОВКИ ИОНАМИ He И H<sub>2</sub> ПОВЕРХНОСТИ АВТОЭМИТТЕРОВ

А.А. Мазиллов

Приводятся аналитическое рассмотрение и численные расчеты параметров, описывающих условия эксплуатации полевых электронных эмиттеров и спектры ионной бомбардировки эмитирующей поверхности. На основании анализа полученных энергетических спектров рассчитана зависимость средней энергии бомбардирующих ионов гелия и водорода от радиуса кривизны эмиттера в процессе отбора автоэлектронного тока и предложена аналитическая аппроксимация результатов.

## ВИЗНАЧЕННЯ СПЕКТРІВ БОМБАРДУВАННЯ ІОНАМИ He І H<sub>2</sub> ПОВЕРХНІ АВТОЕМІТЕРІВ

О.О. Мазілов

Приводяться аналітичний розгляд і чисельні розрахунки параметрів, що описують умови експлуатації польових електронних емітерів і спектри іонного бомбардування поверхні, що емітує. На підставі аналізу отриманих енергетичних спектрів розрахована залежність середньої енергії бомбардуючих іонів гелію й водню від радіуса кривизни емітера в процесі відбору автоелектронного струму та запропонована аналітична апроксимація результатів.