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# Mathematical modeling of the main characteristics of cold field and thermal field electron cathodes of scanning electron microscopes in the study of biological samples

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Main emission characteristics of thermal field and cold field electron cathodes were calculated. Emitters surface forms are approximated by second-order surfaces and anodes are approximated by equipotential surfaces. Systems, consisting of 18 first order ordinary differential equations, are solved using the numerical Runge–Kutta method. As a result, trajectories of the „boundary" electrons were obtained, which determine beam shapes and sizes and density distributions charges and electric field strengths. Analysis of beam parameters let to determine special properties of scanning electron microscopes with thermal field electron cathodes and with cold field electron cathodes for studying biological samples.

**Keywords:** Emission characteristics, mathematical modeling, the cold field electron cathode, the thermal field electron cathode, a scanning electron microscope.

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At present, the use of electro-optical systems based on thermofield and field electron cathodes (TPEC and PEC) is the most promising in the study of the surface, morphology of biosamples for the diagnosis and therapy of diseases. For example, scanning electron microscopy (SEM) is increasingly used in the study of the causes of diseases and the molecular and cellular mechanisms of pathology [1,2]. For example, in studies of the morphology of erythrocytes in patients with cervical cancer (CC) using the SEM method, nanometer objects were found on the surface of erythrocytes of dry blood smears, the identification of which, according to the authors, would contribute to solving the problem of determining the causes of cervical cancer recurrences and the phenomenon of metastasis, as well as to the development of methods for early diagnosis [3]. Identification of nanoobjects using SEM requires an improvement in image quality, which could be achieved by obtaining electron beams of SEM with characteristics suitable for the study of the morphology of biological samples. To do this, it is necessary to develop mathematical models of electronic devices based on cathodes and electron beam control systems with different volt-ampere characteristics of the cathode depending on the parameters of the electric field and electromagnetic lenses, considering the shape and size of injectors and the spatial charge of the electron beam.

In this paper, the emission characteristics of FEC and TFEC are calculated on the basis of the results of numerical experiments conducted on the basis of mathematical models of their main emission characteristics.

The most commonly used injection systems are a diode structure, which consists of a source of charged particles (cathode) and an object of action (anode). Such a system is the simplest electrostatic accelerator, in which, due to the application of a potential difference between the cathode and the anode, a stream of particles with the required energy is obtained. The SEM electron beams are focused by a magnetic field to reduce beam aberration. Electromagnetic lenses, which are wire coils, are used as a focusing system.

In this electron optics problem for calculating the emission characteristics of FEC [4] and TFEC, the surface shape of the emitters is approximated by the second-order surface — ellipsoid of rotation, and the anode — part of the equipotential surface. When building the physical and mathematical models of field and thermofield diodes, the influence of the spatial charge of the beam on the characteristics of diodes is considered. In these models, the influence of the external magnetic field, which controls and focuses the electron beam, is also considered. In the presented models, the electric field plays a dual role: firstly, in both cases it accelerates electrons, secondly, in the case of TFEC it reduces the output of electrons, and in the case of FEC it causes the emission of electrons from the surface of the cathode. For simulation, the concept of „of the outermost " electron is also introduced, the trajectory of which determines the shape and size of the beam.

Thus, the problems of calculating the emission characteristics of ellipsoidal TFEC and FEC, determining the shape and size of the trajectories of outermost electrons are solved using mathematical models that include the following equations: the motion of the outermost electron, Maxwell, continuity, Richardson–Dashmann, considering the Schottky effect in the case of TFEC and Fowler–Nordheim in the case of FEC, as well as the conditions at the beam–vacuum boundary for the outermost electrons:

1) equation of motion of the outermost electron

$$m\ddot{\mathbf{r}}_V = e\mathbf{E}^V + e[\dot{\mathbf{r}}_V, \mathbf{B}];$$

2) the corresponding Maxwell's equations

$$\operatorname{rot}\mathbf{E}^V = 0, \quad \operatorname{div}\mathbf{E}^V = 0;$$

where $m$, $e$ — mass and charge of the electron, respectively, $\mathbf{E}^V$ — electric field strength, $\mathbf{B}$ — induction of the external magnetic field;

3) equation of motion of the outermost electron inside the beam

$$m\ddot{\mathbf{r}} = e\mathbf{E} + e[\dot{\mathbf{r}}, \mathbf{B}];$$

4) the corresponding Maxwell equations

$$\operatorname{rot}\mathbf{E} = 0; \quad \operatorname{div}\mathbf{E} = \frac{\rho}{\varepsilon_0};$$

5) continuity equation:

$$\operatorname{div}\mathbf{j} = 0;$$

6) Richardson–Dashman equation considering the Schottky effect with neglect of the value of the electron reflection coefficient at the body–vacuum boundary (in the case of TFEC)

$$j_0 = A_0 T^2 \exp\left(-\frac{\phi - e\sqrt{eE_0}}{kT}\right),$$

where $\rho$ — the spatial charge density of the emitted electron beam, $j_0$ — current density at the cathode surface, $E_0$ — electric field strength at the cathode surface, $T$ — cathode temperature on the absolute Kelvin scale (K), Sommerfeld thermionic constant:

$$A_0 = \frac{4\pi mek^2}{h^3} = 120.4\,\frac{\mathrm{A}}{\mathrm{cm^2K^2}},$$

$$k = 1.38 \cdot 10^{-23}\ \mathrm{J/K} \text{ — Boltzmann constant,}$$

$$e = 1.6 \cdot 10^{-19}\ \mathrm{C} \text{ — electron charge,}$$

$$\varphi \text{ — electron work function;}$$

7) Fowler –Nordheim equation

$$j_0 = aE_0^2 \exp(-b/E_0),$$

where $j_0$ — current density at the cathode surface, $E_0$ — electric field strength at the cathode surface, $a, b$ — constant values;

8) condition at the boundary beam–vacuum for the outermost electron

$$\frac{\dot{x}_1}{\dot{x}_2} = \frac{\dot{x}_1^V}{\dot{x}_2^V},$$

where $\dot{x}_1^V, \dot{x}_2^V$ — are the components of the charge particle's velocity in curvilinear coordinates outside the beam; $\dot{x}_1, \dot{x}_2$ — components of the electron velocity in curvilinear coordinates inside the beam.

The implementation of the model consists in the joint solution of all these equations of the system, as a result of which the motion of the outermost electron is determined.

In order to decrease the order of the second-order differential equations, new variables for the ellipsoidal cathode are introduced:

$$\xi = \tau\dot{\sigma} + \sigma\dot{\tau},$$

$$\eta = \frac{\sigma\dot{\sigma}}{\sigma^2 - 1} - \frac{\tau\dot{\tau}}{1 - \tau^2}.$$

The model assumes that the diode symmetry axis and the magnetic field have the same direction, i.e. the system under consideration is axially symmetric, and therefore the electric field strength vectors inside and outside the beam, as well as the current density, can be represented as follows, respectively:

$$\mathbf{E} = E_\sigma(\sigma, \tau)\mathbf{e}_\sigma + E_\tau(\sigma, \tau)\mathbf{e}_\tau,$$

$$\mathbf{E}^V = E_\sigma^V(\sigma, \tau)\mathbf{e}_\sigma + E_\tau^V(\sigma, \tau)\mathbf{e}_\tau,$$

$$\mathbf{j} = j_\sigma(\sigma, \tau)\mathbf{e}_\sigma + j_\tau(\sigma, \tau)\mathbf{e}_\tau.$$

In this model, we assume that the coordinate components of the strength and current density vector functions can be considered as the product of functions that depend on only one of the ellipsoidal coordinates $\sigma$, $\tau$.

In this case, the electric field strength inside and outside the beam in ellipsoidal coordinates is as follows:

$$\mathbf{E} = \frac{F_\sigma(\sigma)G_\sigma(\tau)}{(\sigma^2 - \tau^2)^{1/2}}\,\mathbf{e}_\sigma + \frac{F_\tau(\sigma)G_\tau(\tau)}{(\sigma^2 - \tau^2)^{1/2}}\,\mathbf{e}_\tau,$$

$$\mathbf{E}^V = \frac{F_\sigma^V(\sigma)G_\sigma^V(\tau)}{(\sigma_V^2 - \tau_V^2)^{1/2}}\,\mathbf{e}_\sigma + \frac{F_\tau^V(\sigma)G_\tau^V(\tau)}{(\sigma_V^2 - \tau_V^2)^{1/2}}\,\mathbf{e}_\tau,$$

where $F_\sigma, G_\sigma, F_\tau, G_\tau, F_\sigma^V, G_\sigma^V, F_\tau^V, G_\tau^V$ — are the components of the coordinate components of the electric field strength vector inside and outside the beam, respectively, in ellipsoidal coordinates $\sigma, \tau$.

To solve the systems of equations, the following expressions are used for the coordinate components of the current density:

$$\mathbf{j}_\sigma = \frac{f_\sigma(\sigma)g_\sigma(\tau)}{(\sigma^2 - \tau^2)^{1/2}}, \quad \mathbf{j}_\tau = \frac{f_\tau(\sigma)g_\tau(\tau)}{(\sigma^2 - \tau^2)^{1/2}},$$

where $f_\sigma, g_\tau, \sigma_V, \tau_V$ — are the components of the coordinate components of the current density in ellipsoidal coordinates $\sigma, \tau$.

Thus, a closed system of 18 ordinary differential equations with 18 unknowns is obtained: $\sigma$, $\tau$, $\xi$, $\eta$, $F_\sigma$, $G_\sigma$, $F_\tau$, $G_\tau$, $f_\sigma$, $g_\tau$, $\sigma_V$, $\tau_V$, $\xi_V$, $\eta_V$, $F_\sigma^V$, $G_\sigma^V$, $F_\tau^V$, $G_\tau^V$ for ellipsoidal TFEC:

$$\dot{\sigma}_V = \frac{\sigma_V^2 - 1}{\sigma_V^2 - \tau_V^2}\left(\xi_V\tau_V + \eta_V\sigma_V(1 - \tau_V^2)\right),$$

$$\dot{\tau}_V = \frac{1-\tau_V^2}{\sigma_V^2-\tau_V^2}\left(\xi_V\sigma_V - \eta_V\tau_V(\sigma_V^2-1)\right),$$

$$\dot{\xi}_V = \frac{e}{am(\sigma_V^2-\tau_V^2)}\left(\tau_V(\sigma_V^2-1)^{1/2}F_\sigma^V G_\sigma^V + \sigma_V(1-\tau_V^2)^{1/2}F_\tau^V G_\tau^V\right),$$

$$\dot{\eta}_V = K_V + \frac{e}{am(\sigma_V^2-\tau_V^2)}\left(\frac{\sigma_V}{(\sigma_V^2-1)^{1/2}}F_\sigma^V G_\sigma^V - \frac{\tau_V}{(1-\tau_V^2)^{1/2}}F_\tau^V G_\tau^V\right) - \eta_V^2,$$

$$\dot{F}_\tau^V = \frac{c_2}{(\sigma_V^2-1)^{1/2}}F_\sigma^V\dot{\sigma}_V,$$

$$\dot{G}_\sigma^V = \frac{c_2}{(1-\tau_V^2)^{1/2}}G_\tau^V\dot{\tau}_V,$$

$$\dot{F}_\sigma^V = \left(\frac{c_3}{(\sigma_V^2-1)^{1/2}}F_\tau^V - \frac{\sigma_V}{\sigma_V^2-1}F_\sigma^V\right)\dot{\sigma}_V,$$

$$\dot{G}_\tau^V = \left(-\frac{c_3}{(1-\tau_V^2)^{1/2}}G_\sigma^V + \frac{\tau_V}{(1-\tau_V^2)^{1/2}}G_\tau^V\right)\dot{\tau}_V,$$

$$\dot{\sigma} = \frac{\sigma^2-1}{\sigma^2-\tau^2}\left(\xi\tau + \eta\sigma(1-\tau^2)\right),$$

$$\dot{\tau} = \frac{1-\tau^2}{\sigma^2-\tau^2}\left(\xi\sigma - \eta\tau(\sigma^2-1)\right),$$

$$\dot{\xi} = \frac{e}{am(\sigma^2-\tau^2)}\left(\tau(\sigma^2-1)^{1/2}F_\sigma G_\sigma + \sigma(1-\tau^2)^{1/2}F_\tau G_\tau\right),$$

$$\dot{\eta} = K + \frac{e}{am(\sigma^2-\tau^2)}\left(\frac{\sigma}{(\sigma^2-1)^{1/2}}F_\sigma G_\sigma - \frac{\tau}{(1-\tau^2)^{1/2}}F_\tau G_\tau\right)\eta^2,$$

$$\dot{G}_\sigma = \frac{c_4 G_\tau}{(1-\tau^2)^{1/2}}\dot{\tau},$$

$$\dot{F}_\tau = \frac{c_4 F_\sigma}{(\sigma^2-1)^{1/2}}\dot{\sigma},$$

$$\dot{G}_\tau = \frac{G_\sigma\dot{\tau}}{2(1-\tau^2)^{1/2}}\left(\frac{f_\sigma g_\sigma(\sigma^2-1)^{1/2}}{\varepsilon_0\dot{\sigma}F_\tau G_\sigma} - \frac{F_\sigma}{F_\tau}\frac{\sigma}{(\sigma^2-1)^{1/2}} - \frac{G_\tau}{G_\sigma}\frac{\tau}{(1-\tau^2)^{1/2}} - \frac{B_3}{\dot{\sigma}}\right),$$

$$\dot{F}_\sigma = \frac{F_\tau\dot{\sigma}}{2(\sigma^2-1)^{1/2}}\left(\frac{f_\sigma g_\sigma(\sigma^2-1)^{1/2}}{\varepsilon_0\dot{\sigma}F_\tau G_\sigma} - \frac{F_\sigma}{F_\tau}\frac{\sigma}{(\sigma^2-1)^{1/2}} - \frac{G_\tau}{G_\sigma}\frac{\tau}{(1-\tau^2)^{1/2}} + \frac{B_3}{\dot{\sigma}}\right),$$

$$\dot{f}_\sigma = \frac{c_1 f_\sigma\dot{\tau}}{g_\tau(1-\tau^2)^{1/2}}\frac{A_0T^2}{f_\sigma(\sigma_0)} \times \exp\left(-\frac{\phi(\sigma_0^2-\tau^2)^{1/4} - e\sqrt{eF_\sigma(\sigma_0)G_\sigma(\tau)}}{(\sigma_0^2-\tau^2)^{1/4}kT}\right) \times(\sigma_0^2-\tau^2)^{1/2} - \frac{\sigma}{\sigma^2-1}f_\sigma\dot{\sigma},$$

$$\dot{g}_\tau = \left(\begin{array}{l} -\frac{c_1}{(1-\tau^2)^{1/2}}\frac{A_0T^2}{f_\sigma(\sigma_0)} \\ \times\exp\left(-\frac{\phi(\sigma_0^2-\tau^2)^{1/4}-e\sqrt{eF_\sigma(\sigma_0)G_\sigma(\tau)}}{(\sigma_0^2-\tau^2)^{1/4}kT}\right) \\ \times(\sigma_0^2-\tau^2)^{1/2} + \frac{\tau}{(1-\tau^2)^{1/2}}g_\tau \end{array}\right)\dot{\tau},$$

where $c_1, c_2, c_3, c_4$ — constants defined from the initial conditions.

The resulting systems, consisting of 18 ordinary first-order differential equations, are solved using the Runge–Kutta numerical method and calculated parameters whose values comply the requirements for the study of biological samples.

The presented models make it possible to obtain the emission characteristics of TFEC and FEC that are closest to the real ones, inasmuch as the shapes of cathodes are considered by approximating them with a second-order surface, the spatial charge, as well as the effect of an external magnetic field on the electron beam. As a result of the calculation of systems of differential equations, the trajectories of the outmost electrons are obtained, which determine the shape and size of the beams, the distribution of charge densities and the strengths of electric fields.

The obtained theoretical results can be used to create emitters with specified parameters used in solving a wide range of problems, including the study of biological samples. The results make it possible „to control“ the properties of the emitting surface when creating TFEC, FEC with the required parameters, to restore their initial characteristics in case of violation of manufacturing technologies.

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### Conflict of interest

The authors declare that they have no conflict of interest.

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