DOI 10.31489/2022No3/91-96

UDC 537.534.3; 004.942

FOCUS CPM SOFTWARE FOR TRAJECTORY ANALYSIS OF REAL AXIALLY SYMMETRIC ELECTROSTATIC MIRRORS: METHODS AND ALGORITHMS

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The problem of studying the influence of electron mirrors design features, in particular, the gaps between the electrodes on their electron-optical characteristics is solved. A method to solve the problem that combines the advantages of analytical paraxial and numerical approaches is described. FOCUS CPM software developed by the authors of the work that implements the method described is presented. Calculation accuracy is estimated using the example of a three-electrode mirror. A focus position as a function of gap width between cylindrical electrodes is calculated and analyzed.

Keywords: electron optics, paraxial optics, electron mirror, numerical methods, trajectory analysis.

Introduction

A theoretical basis for modern analytical instrumentation is electron optics. The success in the use of mathematical tools to design precision electron- and ion-optical systems is reflected in the achievement of record-breaking parameters of diagnostic equipment: mass spectrometers, electron spectrometers, electron microscopes, micro-computer X-ray tomographs, etc.

Two approaches in modeling systems of electronic and ion optics are widely used: numerical and analytical. A numerical approach makes it possible to carry out a high-precision analysis of system parameters with almost arbitrary configuration of electrodes. Complex real systems are studied with high accuracy by numerical methods. SIMION [1], CPO [2], FOCUS [3] and other software for numerical-solution of electron optics problems are known and widely used in practice. In contrast to solving problems of analysis, the possibilities of synthesizing new designs by numerical methods are severely limited. Synthesis problems are effectively solved using the mathematical apparatus of classical paraxial electron optics.

One of the areas in mass spectrometry of matter is associated with the development of multielectrode mirrors [4], which have unique focusing properties in temporal and spatial domains. The designs of such mirrors are successfully developed using the analytical methods of paraxial optics [5]. But since an analytical expression of potential distribution function is used when designing systems in paraxial approximation, some important issues remain unresolved. Firstly, these are uncontrolled errors in calculating output electron-optical characteristics of real (not idealized) electron mirrors, secondly, the impossibility of taking into account the influence of edge fields, and thirdly, fundamental restrictions on design complexity.

The aim of this work is to combine the advantages of numerical and analytical approaches to the design of electronic mirror schemes. The technique presented here uses the unique analytical approach developed earlier by the authors [5] to the synthesis and optimization of electron-optical parameters of mirrors, but already under conditions of high-precision numerical simulation of electrostatic field. Along with the development of a technique for synthesizing electron mirror schemes, the practical problem of developing a ready-made tool for such synthesis, FOCUS CPM software, is solved.

1. Analytical modeling of paraxial mirrors

The essence of analytical approach in the modeling of electron lenses, mirrors, etc. is to find partial solutions to the basic equation of paraxial optics. Knowing the partial solutions of the equation is the clue to calculating all electron-optical characteristics of the simulated system. In particular, cognition of particular

solutions makes it possible to construct a general solution (the trajectory of central particle), to define cardinal elements of an electron-optical system, and so on.

The paraxial equation in the case of axial symmetry has the form

$$\Phi r" + \frac{1}{2}\Phi' r' + \frac{1}{4}\Phi" r = 0, \tag{1}$$

where $\Phi = \Phi(z)$ is axial distribution of a potential, and the primes denote differentiation with respect to z. Equation (1) is an ordinary linear differential equation of the second order, therefore, it has two linearly independent partial solutions $p=p(z)$ and $g=g(z)$, which form a fundamental system of solutions, the linear combination of which allows us to find a general solution (trajectory equation)

$$r(z) = ap(z) \pm bg(z), \tag{2}$$

where a and b are arbitrary constants determined from the initial conditions in the initial (subject) plane $z=z_0$:

$$a = -\frac{2\sqrt{\Phi_0}}{\Phi'_u}(g_0 r'_0 - g'_0 r_0),$$
$$b = \frac{2\sqrt{\Phi_0}}{\Phi'_u}(p_0 r'_0 - p'_0 r_0), \tag{3}$$

and indices "0" and "u" mark functions values in the plane $z=z_0$ and in the turning plane $z=z_u$, for which $\Phi(z_u)=0$ and $\Phi'(z_u)\neq 0$. In formula (2), sign "+" refers to a direct path branch, and sign "-" refers to a reverse one.

As for the fundamental system of solutions, one of the solutions $p=p(z)$ is an analytic function that satisfies equation (1), which we rewrite as

$$\Phi p" + \frac{1}{2}\Phi' p' + \frac{1}{4}\Phi" p = 0, \tag{4}$$

and the solution g=g(z) can be represented as [5]

$$g(z) = \sqrt{\Phi(z)}q(z), \tag{5}$$

where $q=q(z)$ is an analytic function that satisfies the equation

$$\Phi q" + \frac{3}{2}\Phi' q' + \frac{3}{4}\Phi" q = 0. \tag{6}$$

In the case of electronic mirrors, the functions $p=p(z)$ and $q=q(z)$ must satisfy the following initial conditions [5]

$$p_u = q_u = 1, p'_u = q'_u = -\frac{\Phi''_u}{2\Phi'_u}. \tag{7}$$

The fulfillment of the following equality for the Wronsky determinant

$$W = \sqrt{\Phi(z)}[p(z)g'(z) - p'(z)g(z)] = \frac{1}{2}\Phi'_u \tag{8}$$

is a guarantee of linear independence of solutions.

Within the framework of the analytical approach, a more or less accurate approximation of electric field axial distribution is used as a function $\Phi(z)$, most often expressed by a combination of elementary mathematical functions.

Formula (2) describes the trajectory of the particle launched from a point with coordinates z_0, r_0 at an angle α_0 ($tan(\alpha_0) = r'_0$) with energy $E_0 = \Phi_0$.

As we have already noted, particular solutions make it possible to find cardinal elements of electron mirror [5]. The position of mirror focus and its focal length are determined by equalities

$$z_F = \frac{1}{2}(z_V + z_C), f = \frac{1}{2}(z_V - z_C), \tag{9}$$

where z_V and z_C are vertex coordinates and center of mirror curvature which can be determined from the following considerations. In case when an object and its image are placed in field-free space, particular solutions $p=p(z)$ and $g=g(z)$ are linear functions and therefore can be written as

$$p = (z - z_C)p', g = (z - z_V)g'. \tag{10}$$

Using the fact that the plane $z=z_0$ is located outside the field, from (10) we obtain the desired values

$$z_C = z_0 - \frac{p'_0}{p_0}, z_V = z_0 - \frac{g'_0}{g_0}. \tag{11}$$

2. Algorithm for Numerical Simulation

Numerical approach to solving the problem under consideration methodologically repeats the abovementioned analytical one. The fundamental difference lies in the fact that the function $\Phi(z_i)$ calculated in the array of nodes z_i by the Boundary Element Method [6] is used here as the axial distribution of the potential $\Phi(z)$. This method of determining $\Phi(z)$ is a guarantee of high simulation accuracy and, most importantly, allows one to study the systems with almost arbitrary electrode configuration. The first $\Phi'(z)$, the second $\Phi''(z)$ and the third $\Phi'''(z)$ (we will need it later) derivatives are also spline approximations of corresponding derivatives found at nodes z_i using numerical differentiation formulas [7]. We should note that in standard approaches to the numerical solution of a field problem, the potential distribution and its gradient must be calculated over the entire working region of an electron-optical system [8, 9].

Another advantage of the approach proposed lies in the fact that the trajectory analysis of simulated systems is based on the numerical solution of paraxial equation (1) and finding particular solutions $p=p(z)$ and $g=g(z)$, which in turn allow us to estimate a wide a set of electron-optical characteristics. Here we note that standard non-paraxial numerical methods represent as a result only particle trajectories in the form of a numerical set of two-dimensional coordinates.

A detailed algorithm for electron mirrors numerical simulation in paraxial approximation is as follows. Having found spline approximations of axial distribution of the potential $\Phi(z)$ we are capable to find turning plane position $z=z_u$ by solving the equation

$$\Phi(z_u)=0. \tag{12}$$

Numerical integration by the Runge-Kutta method of equations (4) and (6), written in the form

$$p'' = f_1(z,p,p'), \tag{13}$$

$$q'' = f_2(z,q,q'), \tag{14}$$

taking into account initial conditions (7) allows finding paraxial equation particular solutions $p(z)$ and $g(z) = \sqrt{\Phi(z)}q(z)$ (see (5)).

Integration is performed from the starting point $z=z_u$ with a negative integration step. In the vicinity of this point $z=z_u$ on the right side of equations (13) and (14) there is a singularity (uncertainty of type 0/0), however, removable. After elimination of the singularity, right-hand sides take the forms

$$f_1(z,p,p') = p'^2(z) - \frac{1}{6}\frac{\Phi'''(z)}{\Phi'(z)}, \quad z \to z_u, \tag{15}$$

$$f_2(z,q,q') = \frac{9}{5}\left(q'^2(z) - \frac{1}{6}\frac{\Phi'''(z)}{\Phi'(z)}\right), z \to z_u. \tag{16}$$

When moving away from the singular point, i.e. when the condition $|z - z_u| > \varepsilon$ is satisfied, regular expressions are used as the right parts (see (4) and (6)

$$f_1(z,p,p') = -\frac{2\Phi'(z)p'(z) + \Phi''(z)p(z)}{4\Phi(z)}, \tag{17}$$

$$f_2(z,q,q') = -\frac{6\Phi'(z)q'(z) + 3\Phi''(z)q(z)}{4\Phi(z)}. \tag{18}$$

Here ε is some small value, which, as calculation practice shows, can be quite large. In numerical integration, it suffices to take one first step, at which right-hand sides are calculated using special formulas (15) and (16). After finding particular solutions, the particle trajectory (2) is constructed as a set of forward and backward branches, and focus position and focal length (9) are determined.

3. "FOCUS CPM" software

FOCUS CPM author's software is designed to simulate axially symmetric electron mirrors with almost arbitrary configuration of electrodes in paraxial approximation. The software consists of several modules (graphic editor, electric field calculation module, trajectory analysis modules), the exchange of information between which is carried out using data files.

3.1 Graphic editor (Design)

Graphics editor module is designed to form the meridional section of electrode system with the supply of appropriate potentials to them. The cross section of each electrode is represented as a closed contour oriented counterclockwise with respect to any of its internal points. At the stage of formation, an electrode

can be formed as a combination of the following elements: straight line segments, arcs of circles, parabolas, hyperbolas, ellipses and splines.

3.2 *Module for calculating potential distribution function (FieldE)*.

The module implements the Boundary Element Method (BEM) with the technique developed for calculating singular and quasi-singular integrals [6]. Based on BEM, external Dirichlet problem is solved, which, unlike internal Dirichlet problem, makes it possible to simulate EOS, the designs of which are as close as possible to real ones [8].

The ability to simulate electron-optical systems with the elements of different scales (for example, in case of small gaps between extended electrodes) is another advantage of BEM, in contrast to widely used finite difference methods (FDM) and finite element methods (FEM). In addition, BEM requires no calculation of potentials at all points of a discrete grid covering the simulated area, and allows you to get potential distribution in any subdomain, for example, on the axis of the system.

3.3 *Module for modeling the trajectories of charged particles (PathS).*

The module makes it possible to calculate the set of trajectories of positively charged particles emitted either by a point or by an extended source in a certain range of initial angles (see (2), (3)). Based on the results of calculating the trajectory of a central particle, cardinal elements of electron mirror (9) are calculated.

4 Simulation results

To begin with, the accuracy of path calculations in FOCUS CPM was assessed using the example of modeling the parameters of classical electron lenses with rotational symmetry. It is known [10] that the optical power of weak lenses is represented by an integral of some combination of axial potential distribution function and its derivative. It was noted in [10] that precise calculations are performed with the help of different techniques, also the comparison with the results of numerical simulations show that a given integral expression approximates the optical power of weak lenses with surprisingly good accuracy. The comparison of the results of einzel and immersion lenses optical power calculation using FOCUS CPM software and the integral expression mentioned above showed their guaranteed coincidence within 1%.

One of the ways to significantly increase the resolution of time-of-flight mass spectrometers [11] is the use of electrostatic mirrors of rotational symmetry, e.g., three-electrode ones [5], whose electrodes are coaxial cylinders with equal diameters. In [5], the modes of operation of such mirrors were studied in detail. However, since the authors routinely used an analytical expression of axial potential for an infinitely small gap between cylindrical electrodes, the question for the influence of actual dimensions of these gaps remained open. FOCUS CPM software makes it possible to quantify this impact.

Fig. 1 shows ion-optical scheme of a three-electrode mirror containing all sizes and potentials necessary for modeling. It demonstrates also the picture of electrostatic field equipotentials and a central particle path for “parallel-point” mode of the mirror in case of small but finite gap between the electrodes $\Delta=0.0002d$, where d is the inner diameter of cylinders.

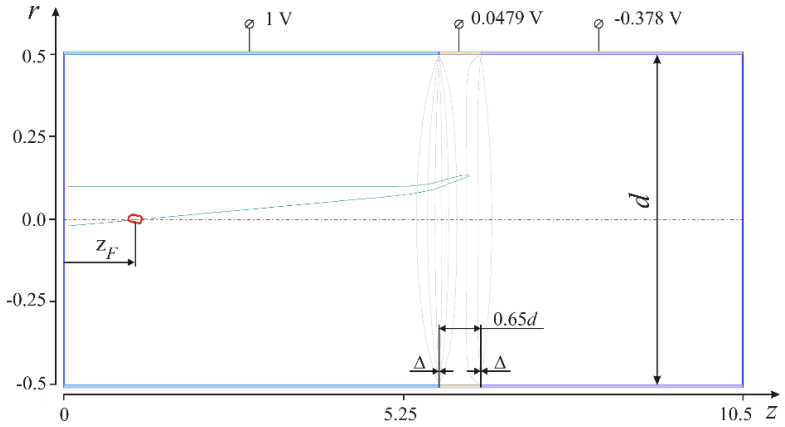

Fig.1. Ion-optical scheme of a three-electrode mirror: results of FOCUS CPM trajectory analysis

Fig. 2 shows the axial distribution of the potential $\Phi(z)$, as well as its first $\Phi'(z)$ and second $\Phi''(z)$ derivatives. The focus position, in accordance with (9), turns out to be equal to $z_F = 1.18d$. The results

obtained in FOCUS CPM when modeling mirrors were additionally verified using FOCUS Pro software [3] developed for numerical analysis of real (not paraxial) EOS/IOS. Once again, we note that in this case it is necessary to calculate the field in the entire working area of EOS and a set of particle trajectories. Fig. 3 shows the results of calculation for 10 particle trajectories in the mirror with $\Delta=0.0002d$ having different radial start coordinates r. Based on the set of trajectories, the position and the order of spatial focus are estimated using a numerical method [12]. The result of the estimate is as follows: a mirror provides second-order focusing in terms of the initial coordinate r at the point $z_F = 1.12d$. To be able to conduct a comparative analysis, the results of calculations of the focus position z_F by different methods are collected in Table 1.

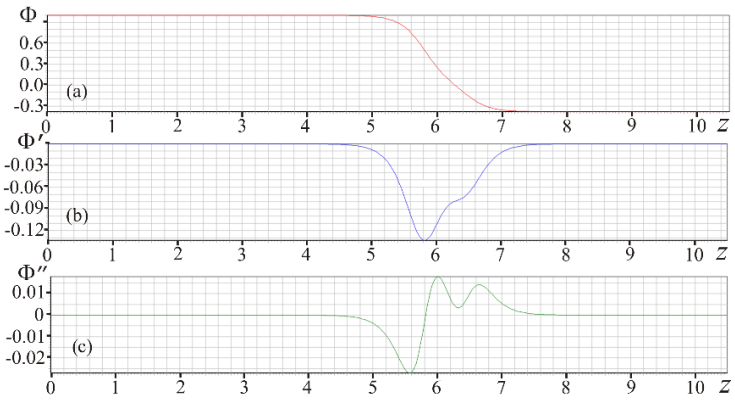

Fig.2. Axial distributions of (a) the potential Φ(*z*), (b) the first Φ'(*z*) and (c) the second Φ"(*z*) derivatives of the potential in a three-electrode mirror

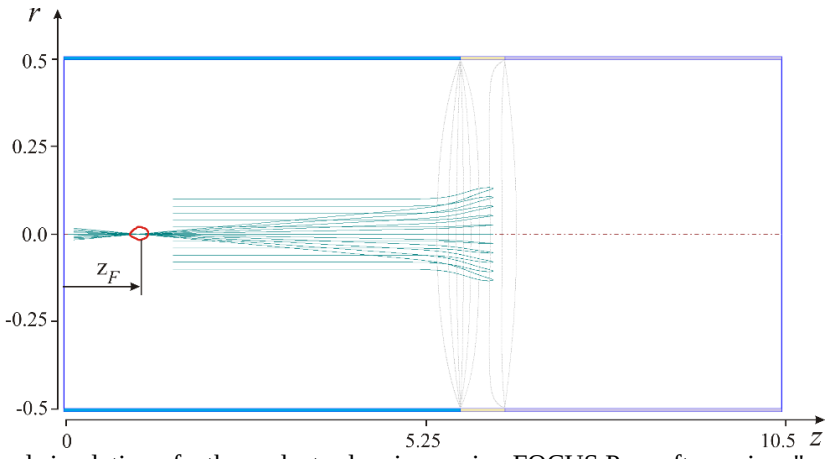

Fig.3. Results of numerical simulation of a three-electrode mirror using FOCUS Pro software in a "parallel-point" mode

Table 1. Focus position z_F

	Method		
	Analytical	FOCUS CPM	FOCUS Pro
Position z_F	1.01d	1.18d	1.12d

An analysis of tabular data allows us to conclude that the error in calculating the parameters of an electron mirror in the case of an analytical expression of the potential [5] is about 10%; while the numerical solution of field problem improves calculation error by about an order of magnitude. At the same time, the time for solving the problem in a paraxial approximation by means of new FOCUS CPM software is reduced by thousands of times compared to the case of using FOCUS Pro numerical simulation software [3]. In terms of its main characteristics (counting speed and accuracy), the FOCUS CPM software presented is ideal for optimizing designs, e.g., electronic mirrors and studying the effect of their geometric features on output electron-optical parameters. Fig. 4 demonstrates the dependence of a focus position z_F on the size of a gap between cylindrical electrodes Δ, which must be taken into account when manufacturing a real device.

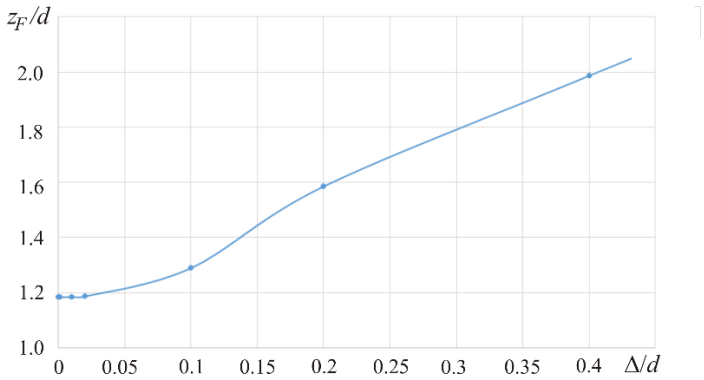

Fig. 4. Dependence of a focus position on the size of a gap between cylindrical electrodes

It follows from the last dependence that in the range of small gaps up to about 5% of *d*, a focus position is almost constant and approximately doubles with a further increase in the gap to 40% of *d*.

Conclusion

In this paper for the first time a unique analytical technique for modeling the parameters of multielectrode electron mirrors [5] is combined with an original technique for numerical solution of an external field problem using the Boundary Element Method [6, 8]. The developed approach implemented in the form of FOCUS CPM software application makes it possible to design electron mirrors with a practically arbitrary electrode configuration at a high counting rate. The high accuracy (on the order of a few percent) of the calculations of charged particle trajectories and electron-optical parameters of multielectrode mirrors in FOCUS CPM is established. A practically important dependence of a focus position on the size of a gap between the electrodes is obtained for a three-electrode mirror.

Acknowledgments

This research has been funded by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. AP08855808).

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Article accepted for publication 26.07.2022