TIME-OF-FLIGHT MASS ANALYZER BASED ON TRANSAXIAL MIRRORS*

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The motion of charged particles emerging from a point source located in the middle plane of the transaxial mirror is considered. It is shown that as a result of reflection in a three-electrode transaxial mirror, a parallel volume beam can be formed. To calculate the trajectories of particles, the dimensionless Newton equations and analytical expressions for the potential are used, which describe the field of a three-electrode transaxial mirror with good accuracy. Two modes of vertical beam focusing are calculated. The transaxial mirrors can be used to create highly efficient time-of-flight mass spectrometers.

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1. Introduction

Recently, time-of-flight multi-reflective mass analyzers have been successfully used in various fields of science [1]. In such analyzers, electrostatic mirrors are used, in which it is possible to carry out spatial focusing of the beam in two directions and, at the same time, time-of-flight focusing in terms of ion energy, which makes it possible to achieve mass resolution of $R_m > 1\,000\,000$ with high sensitivity and speed of analysis. In [2], it was proposed to use such a mass analyzer for precision measurement of the masses of superheavy elements resulting from the bombardment of neutron-rich target nuclei with heavy ions. Accurate measurement of the masses of such nuclei with $Z \geq 115$ may be the key for studying their nuclear structure.

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It is known that when calculating the trajectories of charged particles in electrostatic mirrors, mathematical difficulties arise due to the fact that in the vicinity of the turning points, the radii of curvature of the trajectories tend to zero. In this case, the slopes of the trajectories to the optical axis and the relative spread of particle energies increase indefinitely [3, 4]. All these difficulties remain aside if we integrate not the trajectory equations, but Newton's equations with respect to the time of motion of the particles. Numerical integration of Newton's equations is greatly simplified if the analytical expressions for the potentials describing the electric fields of the mirrors are known. To find the potentials describing the electrostatic fields of corpuscular-optical systems (COS), as a rule, one has to solve the Dirichlet problem for a scalar potential that satisfies the Laplace equation. The potentials of the transaxial COS in the cylindrical coordinate system ρ, ψ, z depend only on the variables ρ and z and satisfy the Laplace equation [5]

$$\frac{\partial^2\varphi}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial\varphi}{\partial\rho} + \frac{\partial^2\varphi}{\partial z^2} = 0\,. \tag{1}$$

The most general method for solving the Dirichlet boundary value problem for equation (1) is the method of separation of variables. In this case, the potentials are represented in the form of a series of Bessel functions [5]. However, these solutions are difficult to use for numerical calculations due to poor convergence of the series. In [6–10], simple approximate analytical expressions were found for the potential of a three-electrode transaxial lens, which also describe the field of a transaxial mirror with good accuracy. Such mirrors can be used, in particular, to create time-of-flight mass spectrometers. The present work is devoted to the calculation of the properties of such mirrors.

2. Analytical expressions for the potential of a transaxial mirror

A three-electrode transaxial lens or mirror consists of two parallel plates cut by straight circular cylinders of radius R_1 and R_2, the axis of which coincides with the axis z [9, 10]. Such a mirror is shown schematically in Fig. 1. The figure also shows the accompanying Cartesian coordinate system x, y, z. The origin of the Cartesian coordinate system is in the median plane of the mirror, which coincides with the plane xy; V_0, V_1, and V_2 are the potentials of the electrodes, d is the distance between the plates. The gaps between the electrodes are considered to be infinitely narrow. Far from the edges of the plates, the potential φ depends only on the variables $\rho = \sqrt{x^2 + y^2}$ and z.

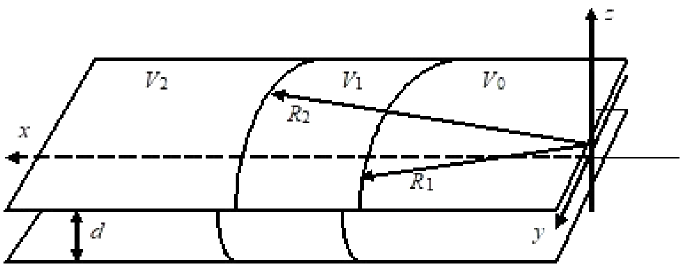

Fig. 1. Schematic representation of a transaxial lens and mirror.

Introducing dimensionless variables [9, 10]

$$\eta = \ln \frac{\rho}{R}, \qquad \zeta = \frac{z}{R}, \tag{2}$$

where $R = \sqrt{R_1 R_2}$, we obtain the following equation for the potential:

$$e^{-2\eta} \frac{\partial^2 \varphi}{\partial \eta^2} + \frac{\partial^2 \varphi}{\partial \zeta^2} = 0\,. \tag{3}$$

The harmonic component $F(\eta, \zeta)$ of the electrostatic potential $\varphi\ (\eta, \zeta)$ satisfies the two-dimensional Laplace equation and is a harmonic function of the dimensionless variables η and ζ. Therefore, for the calculation $F(\eta, \zeta)$, you can use the apparatus of the theory of functions of a complex variable (TFCV) [11]. The analytical expressions obtained in this way for the potential give a good approximation for the potential $\varphi\ (\eta, \zeta)$, since it exactly satisfies the given Dirichlet boundary conditions, and at $\rho \cong R$ ($\eta = 0$) they satisfy the two-dimensional Laplace equation.

In cylindrical coordinates, analytical expressions for the electrostatic potential of three-electrode transaxial lenses can be written in the following form [7, 8]:

$$\varphi\ (\rho, z) = V_2 + (V_0 - V_1)\, P_1 \left(\frac{\rho}{R_1}, z, R \right) + (V_1 - V_2)\, P_2 \left(\frac{\rho}{R_2}, z, R \right), \tag{4}$$

where

$$P_k \left(\frac{\rho}{R_k}, z, R \right) = \frac{1}{\pi} \operatorname{arctg} \frac{2 \cos \frac{\pi}{d} z}{\left(\frac{\rho}{R_k}\right)^{\frac{\pi R}{d}} - \left(\frac{\rho}{R_k}\right)^{-\frac{\pi R}{d}}} \qquad (k = 1, 2)\,. \tag{5}$$

This rather simple analytical expression obtained for the electrostatic potential of a three-electrode transaxial lens can also be used to calculate transaxial mirrors.

3. Dimensionless Newton equations

When studying the dynamics of a beam of charged particles in transaxial mirrors, we will use the dimensionless Newton equations [6]. The equations of motion of a charged particle with charge q and mass m in an electrostatic field in dimensionless Cartesian coordinates x, y, z can be written in the following form:

$$\ddot{x} = \frac{\partial \varphi}{\partial x}\,, \qquad \ddot{y} = \frac{\partial \varphi}{\partial y}\,, \qquad \ddot{z} = \frac{\partial \varphi}{\partial z}\,. \tag{6}$$

Here, the potential φ is measured in units V_0; the unit of length is taken as the distance d between the parallel planes of the transaxial mirror; dots denote derivatives with respect to dimensionless time $\tau = t/\tau_0$, where

$$\tau_0 = d\sqrt{\frac{m}{q\,V_0}}\,. \tag{7}$$

The initial conditions for calculating trajectories when integrating equations (6) can be set as follows:

$$\begin{aligned} x_0 &= a\,, \qquad y_0 = b\,, \qquad z_0 = c\,; \qquad \dot{x}_0 = \sqrt{2(1+\varepsilon) - \dot{y}_0^2 - \dot{z}_0^2}\,, \\ \dot{y}_0 &= \sqrt{2(1+\varepsilon)}\,\sin\alpha\,, \qquad \dot{z}_0 = \sqrt{2(1+\varepsilon)}\,\sin\beta\,. \end{aligned} \tag{8}$$

Here, ε is the relative spread in energy at the entrance to the system; angles α and β determine the angular spread in the beam in the horizontal and vertical directions, respectively. When moving in the middle plane of the mirror, where $z_0 = \dot{z}_0 = 0$, the angle α formed by the beam with the axis x, which is the main optical axis of the mirror, is determined by the expression

$$\mathrm{tg}\,\alpha = \frac{\dot{y}_0}{\dot{x}_0}\,. \tag{9}$$

To calculate the derivatives of the potential included in equations (6), the following formulas are used for the derivatives of the potential determined by expressions (4) and (5):

$$\frac{\partial P_k}{\partial \rho} = -\frac{\frac{2R}{R_k d}\cos\frac{\pi}{d}z\left[\left(\frac{\rho}{R_k}\right)^{\frac{\pi R}{d}-1} + \left(\frac{\rho}{R_k}\right)^{-\frac{\pi R}{d}-1}\right]}{\left[\left(\frac{\rho}{R_k}\right)^{\frac{\pi R}{d}} - \left(\frac{\rho}{R_k}\right)^{-\frac{\pi R}{d}}\right]^2 + 4\cos^2\frac{\pi}{d}z}\,, \tag{10}$$

$$\frac{\partial P_k}{\partial x} = \frac{\partial P_k}{\partial \rho}\frac{\partial \rho}{\partial x} = \frac{\partial P_k}{\partial \rho}\,\frac{x}{\rho}\,, \qquad \frac{\partial P_k}{\partial y} = \frac{\partial P_k}{\partial \rho}\frac{\partial \rho}{\partial y} = \frac{\partial P_k}{\partial \rho}\,\frac{y}{\rho}\,, \tag{11}$$

$$\frac{\partial P_k}{\partial z} = -\frac{\frac{2}{d}\,\sin\frac{\pi}{d}\,z\left[\left(\frac{\rho}{R_k}\right)^{\frac{\pi R}{d}} - \left(\frac{\rho}{R_k}\right)^{-\frac{\pi R}{d}}\right]^2}{\left[\left(\frac{\rho}{R_k}\right)^{\frac{\pi R}{d}} - \left(\frac{\rho}{R_k}\right)^{-\frac{\pi R}{d}}\right]^2 + 4\,\cos^2\frac{\pi}{d}\,z}\,. \tag{12}$$

The given values of the derivatives were substituted into the differentiated expression (4) and thus the right-hand sides of equations (6) were determined.

4. Results of numerical calculation

Dimensionless Newton equations (6) were integrated numerically by the four-point Adams method with an automatic choice of the integration step. The accelerating points were found by the method of successive approaches of Krylov. The relative accuracy of integration was chosen to be equal $10^{-8} \div 10^{-9}$.

Numerical calculations were carried out for a transaxial mirror, for which $R_1 = 10d$, $R_2 = 12d$; $V_0 = 1$, $V_1 > 0$, $V_2 < 0$. The unit of length was chosen as $d = 1$ — the distance between the parallel planes of the transaxial mirror. The initial conditions simulated a point source located in the area outside the field in the median plane of the mirror at the point: $x_0 = 5$, $y_0 = 0.4935$, $z_0 = 0$. The axial trajectory was directed at an angle $\alpha \cong 2^\circ$ to the axis E, by specifying the following initial conditions: $\dot{x}_0 = \sqrt{2 - \dot{y}_0^2}$, where $\dot{y}_0 = -0.0495$. The volumetric beam was modeled by the following changes in the initial conditions: $|\Delta\,\alpha| \le 0.004$ rad, $|\dot{z}_0| \le 0.003$, $|\varepsilon| \le 0.01$. With the indicated changes in the initial conditions, the paraxial approximation is still quite well satisfied.

The calculation results are shown in Figs. 2 and 3. Figure 2 shows the behavior of the beam in projection onto the middle plane of the mirror, and Fig. 3 — the behavior of the extreme trajectories of the beam in the vertical direction. The potentials of the electrodes were selected so that the linear focus in the vertical direction was located symmetrically to the position of the source relative to the axis x. This situation was realized at the following electrode potentials: $V_0 = 1$, $V_1 = 0.51$, $V_2 = -0.05545$. The time of flight of particles to the plane of the detector, which passes through a point $x_k = x_0 = 5$ perpendicular to the axial trajectory of the beam, was also determined. For the axial trajectory ($\varepsilon = 0$), the time of arrival at the detector is equal to $\tau_{d\,0} = 16.3$, and for particles moving along the axial trajectory with a different energy: at $\varepsilon = 0.01$, we get $\tau_{d\,1} = 16.91$, and at $\varepsilon = 0.01$ — $\tau_{d\,2} = 15.89$. It can be seen from these data that there should be a plane where time-of-flight energy focusing and, at the same time, spatial focusing of the beam are carried out.

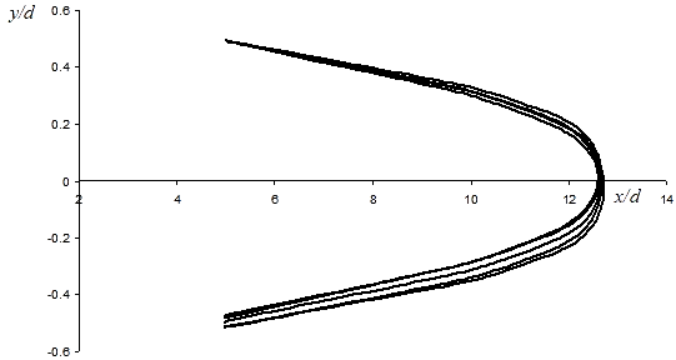

Fig. 2. Projection of the beam onto the middle plane of the mirror.

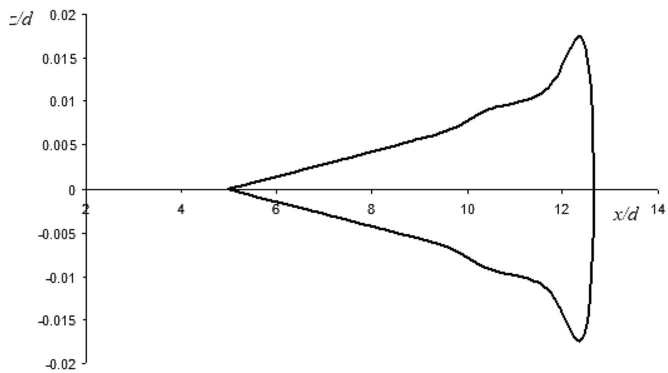

Fig. 3. Projections of the extreme beam paths to the vertical direction.

Dimensionless Newton equations for different initial conditions were integrated over dimensionless time τ to the same final value $\tau_{k0} = \tau_{d0}$. In this case, due to different initial conditions, some particles did not reach the detector plane, and some flew over the detector plane. In this case, the time of arrival of charged particles to the detector was determined taking into account the fact that near the plane of the detector, where the field is absent, the particles move along rectilinear trajectories with a constant velocity. If by the time instant $\tau = \tau_{k0}$ the particle was at the point $(x_k,\, y_k,\, z_k)$ and moved with the speed $(\dot{x}_k,\, \dot{y}_k,\, \dot{z}_k)$, then the distance to the detector plane was found.

The equation of the detector plane passing through the point $(x_d,\, y_d)$ parallel to the axis z is

$$y - y_d = k_d(x - x_d)\,, \tag{13}$$

where $k_d = -1/\mathrm{tg}\,\alpha$. The equation of the projection of the trajectory onto the plane xy can be written as

$$y - y_k = k_k(x - x_k)\,, \tag{14}$$

where $k_k = \dot{y}_k/\dot{x}_k$. Coordinates of the point of intersection of this projection with the detector plane

$$x_1 = \frac{k_k x_k - k_d x_d + y_d - y_k}{k_k - k_d}\,, \qquad y_1 = k_k(x_1 - x_k) + y_k\,. \tag{15}$$

Now the time of arrival at the detector is determined by the formula:

$$\tau_d = \tau_{d\,0} \pm \frac{\sqrt{(x_1 - x_k)^2 + (y_1 - y_k)^2}}{\upsilon_{x\,y}}\,. \tag{16}$$

Here, the sign "+" is taken if the particle does not reach the detector plane, and the sign "−" if it flies over the detector plane; a $\upsilon_{x\,y}$ is the projection of the velocity onto the plane $x\,y$

$$\upsilon_{x\,y} = \sqrt{\dot{x}_k^2 + \dot{y}_k^2}\,. \tag{17}$$

It is also possible to carry out a telescopic behavior of the beam in the vertical direction, slightly changing the potential at the reflecting electrode. If we apply a potential $V_2 = -0.05765$ to it, then at the exit from the mirror we get an almost parallel beam of particles. Figure 4 shows the course of the extreme trajectories of the beam for this case.

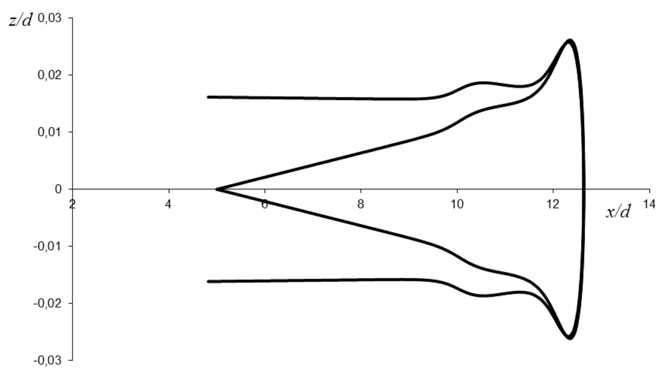

Fig. 4. Projections of the extreme beam paths to the vertical direction.

5. Conclusion

The use of analytical expressions describing the field of transaxial three-electrode mirrors made it possible to numerically integrate Newton's dimensionless equations for a charged particle in the field of a mirror, and thus to study the behavior of a beam of charged particles in a transaxial mirror. It is shown that, as a result of reflection in a transaxial mirror, a diverging beam can be converted into an almost parallel one and high-quality spatio-temporal focusing can be achieved. This property of transaxial mirrors can be used to create highly efficient time-of-flight mass spectrometers consisting of various combinations of transaxial mirrors.

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