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Improved method for designing a cylindrical Zhang–Enke ion mirror

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Abstract

A series solution for the potential within a cylindrical, three-element Zhang–Enke ion mirror has been obtained. The only simplification is that the small gaps between mirror elements are ignored. Automated function minimization by the simplex method has been used to optimize the mirror region lengths and voltages. Flight times only along the central axis were used here for convenience, but the potential can be calculated fully in three dimensions. The mirror designed by this method has good focusing characteristics. Additional refinement could be obtained by optimization of three-dimensional ion trajectories starting from the one-dimensional parameters obtained here. (Int J Mass Spectrom 214 (2002) 89–94) © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

Zhang and Enke described a new type of ion mirror [1–3] which is comprised of only three substantive elements and a single grid which covers the aperture (see Fig. 1). Their theoretical studies indicate that the mirror performance would be at least as good as a conventional two-stage linear-field mirror. Recently such a mirror has been tested in our laboratory, and initial results indicate that the mirror performs as expected, at least as well as a two-grid Mamyrin-style mirror [4].

To design the three-element mirror (that is, to assign values to the lengths a, b, and c, the diameter d, and the voltages V_1 and V_2), Zhang and Enke used the SIMION 3D [1] program to calculate the electrical potential inside the mirror for a set of test parameters and then simulated ion trajectories through it. The test parameters were varied manually using the simplex method [5], then new potential and trajectory simulations were run. Eventually a "best" set of conditions was determined. We have now obtained a series solution for the mirror potential and have developed an automated method for optimization of the mirror parameters.

2. Series solution for the mirror potential

To obtain the potential in the Zhang–Enke mirror, we introduce the following notation related to Fig. 1:

$$z_1 = a, \qquad z_2 = a + b,$$
$$L = a + b + c, \qquad r = \frac{d}{2}.$$

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[1] Scientific Instrument Services, Inc., Ringoes, NJ, USA.

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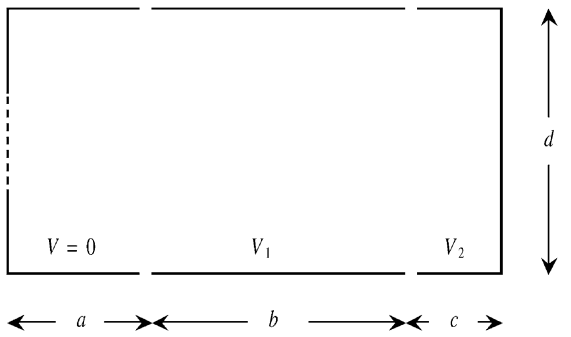

Fig. 1. The Zhang–Enke mirror, containing three cylindrical elements. (Other cross-section shapes are possible as well.)

The z-axis is oriented so that $z = 0$ lies at the entrance grid. The desired potential is the solution to Laplace's equation, shown here in cylindrical coordinates:

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\Phi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\Phi}{\partial\theta^2} + \frac{\partial^2\Phi}{\partial z^2} = 0. \quad (1)$$

For the axially symmetric problem, the potential is independent of θ. Separability of Laplace's equation allows the potential to be written as $\Phi(\rho, z) \equiv R(\rho)Z(z)$, and the partial differential equation to be written as a pair of ordinary differential equations,

$$\frac{\mathrm{d}^2Z}{\mathrm{d}Z^2} - k^2Z = 0 \qquad \frac{\mathrm{d}^2R}{\mathrm{d}R^2} + \frac{1}{\rho}\frac{\mathrm{d}R}{\mathrm{d}\rho} + k^2R = 0, \quad (2)$$

where k^2 is the constant of separation.

The solutions to the ordinary differential equations have the usual form, depending upon the sign of the separation constant, k^2,

$$\text{for } k^2 > 0: \quad Z \sim \left\{\begin{matrix}\sinh kz\\ \cosh kz\end{matrix}\right\}, \quad R \sim \left\{\begin{matrix}J_0(k\rho)\\ N_0(k\rho)\end{matrix}\right\}$$
$$\text{for } k^2 < 0: \quad Z \sim \left\{\begin{matrix}\sin kz\\ \cos kz\end{matrix}\right\}, \quad R \sim \left\{\begin{matrix}I_0(k\rho)\\ K_0(k\rho)\end{matrix}\right\},$$

where $J_0\,(N_0)$ is the zeroth order Bessel function of the first (second) kind, and $I_0\,(K_0)$ is the zeroth order modified Bessel function of the first (second) kind.

The problem is divided into the two sub-problems illustrated in Fig. 2. Linear superposition of solutions is used to find the general solution.

2.1. Sub-problem A—grounded cylinder

Here the potential on the side wall ($\rho = r$) is zero, so the Bessel function $J_0(k_n\rho)$ is required for the radial part of the solution. Also, the potential is zero at $z = 0$, leading to $\sinh(k_nz)$ for the z-dependent part of the solution. The potential takes the form

$$V(\rho, z) = \sum_{n=1}^{\infty} A_n \sinh(k_nz) J_0(k_n\rho) \quad (3)$$

where k_n are the solutions of the determining equation $J_0(k_nr) = 0$; i.e., $k_n = X_{0n}/r$ with X_{0n} the nth root of $J_0(x)$. At the top face, the potential is V_0, thus

$$V(\rho, z = L) = V_0 = \sum_{n=1}^{\infty} A_n \sinh\left(\frac{X_{0n}}{r}L\right) J_0\left(\frac{X_{0n}}{r}\rho\right). \quad (4)$$

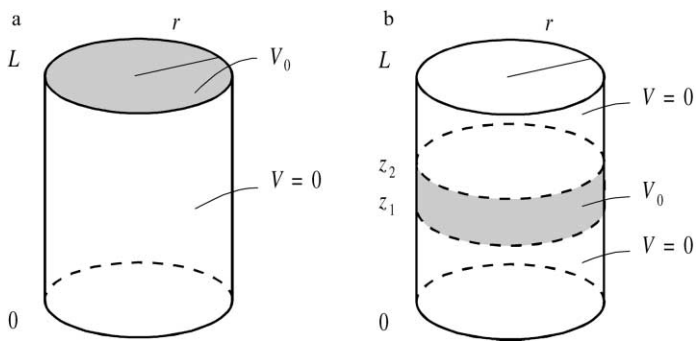

Fig. 2. The two sub-problems and their associated parameters. (a) Grounded cylinder with face at V_0; (b) Interior ring at V_0 with grounded exterior.

To determine the expansion coefficients, Eq. (4) is multiplied by $\rho J_0((X_{0m}/r)\rho)$ and integrated over ρ from 0 to r. The orthogonality of the Bessel functions is used to simply determine the coefficients of the expansion:

$$A_m = \frac{2V_0}{X_{0m}J_1(X_{0m})\sinh((X_{0m}/r)L)}. \quad (5)$$

The solution to sub-problem A is thus given by

$$V(\rho,z) = \sum_{n=1}^{\infty} \frac{2V_0}{X_{0n}J_1(X_{0n})\sinh((X_{0n}/r)L)} \times \sinh\left(\frac{X_{0n}}{r}z\right) J_0\left(\frac{X_{0n}}{r}\rho\right). \quad (6)$$

2.2. Sub-problem B—interior ring

For this configuration, the potentials at $z = 0$ and $z = L$ are zero. The required form for the solution is thus $Z(z) \sim sin(k_n z)$, where $k_n = n\pi/L$. The requirement that the solution be finite at $\rho = 0$ specifies the radial part of the solution to be the modified Bessel function of the first kind. The full solution then has the form

$$V(\rho,z) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi}{L}z\right) I_0\left(\frac{n\pi}{L}\rho\right). \quad (7)$$

At the edge of the cylinder, $V(\rho = r, z) = V_0(z)$,

$$V_0(z) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi}{L}z\right) I_0\left(\frac{n\pi}{L}r\right) \quad (8)$$

where $V_0(z)$ is constant and equal to V_0 for $z_1 < z < z_2$, and zero elsewhere.

To determine the expansion coefficients for this problem, Eq. (8) is multiplied by $\sin(m\pi z/L)$ and integrated over z from 0 to L. The orthogonality of the sine functions is used to simply determine the coefficients of the expansion:

$$A_m = \frac{2V_0[\cos(m\pi z_1/L) - \cos(m\pi z_2/L)]}{m\pi I_0(m\pi r/L)} \quad (9)$$

The solution to sub-problem B is thus given by

$$V(\rho,z) = \sum_{n=1}^{\infty} \frac{2V_0[\cos(n\pi z_1/L) - \cos(n\pi z_2/L)]}{n\pi I_0(n\pi r/L)} \times \sin\left(\frac{n\pi z}{L}\right) I_0\left(\frac{n\pi\rho}{L}\right). \quad (10)$$

2.3. General solution

We combine the results of Eqs. (6) and (10) to obtain the solution for the general problem shown in Fig. 3.

The potential over the entire volume of the structure takes the form

$$V(\rho,z) = \frac{2V_1}{\pi}\sum_{n=1}^{\infty} \frac{(\cos(n\pi z_1/L) - \cos(n\pi z_2/L))}{nI_0(n\pi r/L)} \times \sin\left(\frac{n\pi z}{L}\right) I_0\left(\frac{n\pi\rho}{L}\right) + \frac{2V_2}{\pi}\sum_{n=1}^{\infty} \frac{(\cos(n\pi z_2/L) - (-1)^n)}{nI_0(n\pi r/L)} \times \sin\left(\frac{n\pi z}{L}\right) I_0\left(\frac{n\pi\rho}{L}\right) + 2V_2\sum_{n=1}^{\infty} \frac{\sinh((X_{0n}/r)z)J_0((X_{0n}/r)\rho)}{X_{0n}J_1(X_{0n})\sinh((X_{0n}/r)L)}. \quad (11)$$

The only simplification for this model is that the spacing between the three elements is zero. In practice, there are small gaps, e.g., 1 mm, between elements. These gaps have a negligible effect, however, on the field shape near the axis. An example potential calculated from Eq. (11) is shown in Fig. 4, using parame-

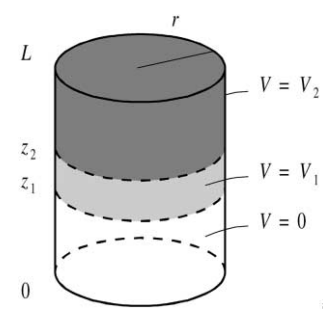

Fig. 3. The general problem and associated terms.

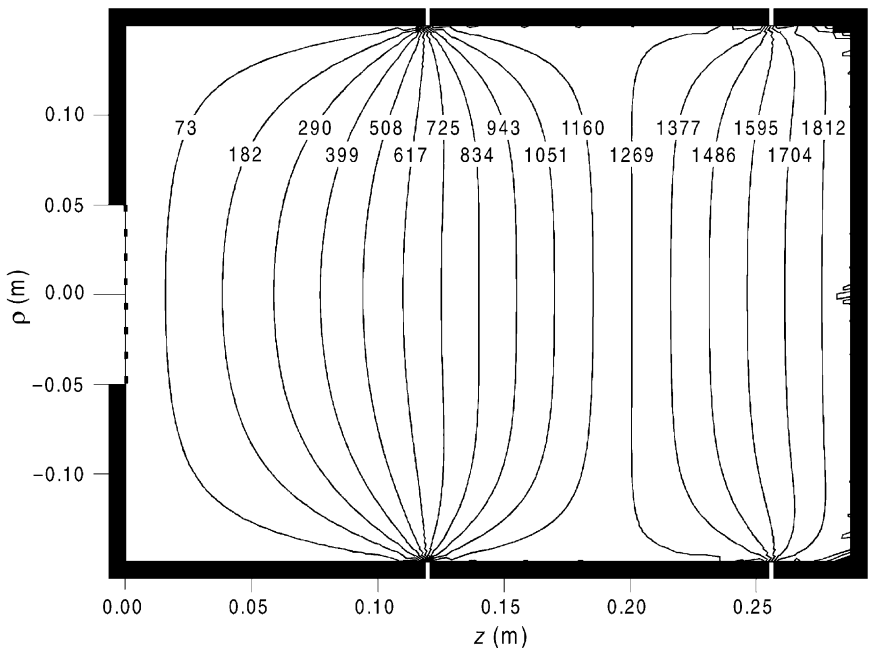

Fig. 4. Potential calculated in the Zhang–Enke mirror with the following parameters: $z_1 = 0.119\,\text{m}$, $z_2 = 0.257\,\text{m}$, $L = 0.288\,\text{m}$, $V_1 = 1247\,\text{V}$, $V_2 = 1897\,\text{V}$, $r = 0.149\,\text{m}$. Mirror element geometry and a grid of (arbitrary) 0.1-m diameter are indicated by thick lines.

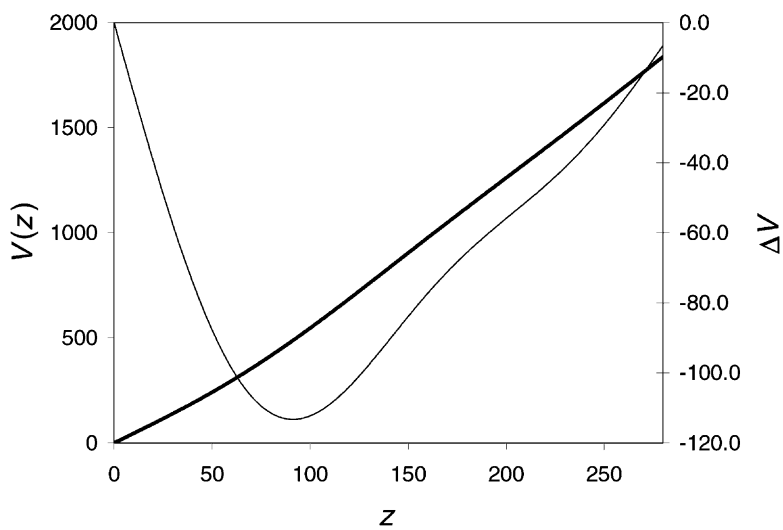

Fig. 5. Potential along the central axis ($\rho = 0$) for the parameters detailed in Fig. 4 (thick line). The thin line shows the deviation from a linear potential, as plotted in ref. [3].

ters matching those published by Zhang and Enke [3]. Note that the solution could be expanded to include additional mirror elements if desired.

To design the mirror segment lengths (a, b, and c) and voltages, we are interested primarily in the field shape along the central axis. Thus, setting ρ to 0 yields the following simplified equation for the potential along the axis:

$$V(z, \rho = 0) = \frac{2V_1}{\pi}\sum_{n=1}^{\infty}\frac{(\cos(n\pi z_1/L) - \cos(n\pi z_2/L)}{nI_0(n\pi r/L)} \times \sin\left(\frac{n\pi z}{L}\right) + \frac{2V_2}{\pi}\sum_{n=1}^{\infty}\frac{(\cos(n\pi z_2/L)) - (-1)^n}{nI_0(n\pi r/L)} \times \sin\left(\frac{n\pi z}{L}\right) + 2V_2\sum_{n=1}^{\infty}\frac{\sinh((X_{0n}/r)z)}{X_{0n}J_1(X_{0n})\sinh((X_{0n}/r)L)}. \quad (12)$$

Numerical evaluation of this expression is substantially more convenient than simulation of the entire field shape by SIMION 3D. The potential calculated from Eq. (12) for the example case is shown in Fig. 5. This plot closely matches the potential reported by Zhang and Enke [3].

3. Optimization of mirror parameters

Ion flight times can be calculated into and out of the mirror field along the central axis using standard numerical integration methods. The flight time is given by

$$T_{\text{mirror}}(v_0) = \sqrt{2m}\int_0^{X_f}\frac{1}{\sqrt{((mv_0^2)/2) - q(V(x))}}\mathrm{d}x. \quad (13)$$

Here v_0 is the initial ion velocity into the mirror, and $V(x)$ is calculated from Eq. (12).

Flight time through the instrument is the sum of flight times through the field-free and mirror regions; thus $T(v_0) = T_{\text{ff}}(v_0) + T_{\text{mirror}}(v_0)$. A properly designed mirror will minimize the deviations in flight time brought about by differing values of v_0. A response function can be defined to indicate "quality" of energy focus. To constrain the system to reasonable size, the total mirror length, L, is fixed. Similarly, V_2 is fixed at the maximum desired voltage. This leads to a three-parameter optimization problem to select values for z_1, z_2, and V_1. We define a response function, $F(\boldsymbol{M})$, as the sum of the squares of flight time deviations for several initial velocities, where $\boldsymbol{M}$ is the vector of mirror parameters $\{z_1, z_2, V_1\}$, as shown in Eq. (14).

$$F(\boldsymbol{M}) = \sum_{i=1}^{n}[(T(v_i, \boldsymbol{M}) - T(v_0, \boldsymbol{M}))^2] \quad (14)$$

Our response function could be extended to include flight times in the ion source or other regions, of course. Typically, physical limits such as negative lengths are avoided by assigning an invalid (e.g., very high) value to $F(\boldsymbol{M})$ for disallowed parameters. Automated simplex optimization or other numerical function-minimization methods can be used to determine the best parameters by finding the minimum value for $F(\boldsymbol{M})$.

Often the choice of starting point for a global minimization problem is difficult. Zhang and Enke's previous work [3] suggested conditions for their optimization procedure, however, which work here as well. In particular, for a system with lowest energy of interest qV_{min} and maximum ion energy of qV_{max}, we begin with the assignments $V_1 = V_{\text{min}}$, $z_1 = L/4$, and $z_2 = 3z_1$. The value for V_2 is fixed at $1.1 \times V_{\text{max}}$.

Once the optimization is accomplished, it would be wise to study flight time with a three-dimensional simulation such as that provided by SIMION 3D in order to observe perturbations caused by field non-uniformities across the mirror diameter. In fact, the best solution is a compromise between our "ideal" field calculated along the central axis and slightly differing fields which bring non-axial ions into focus (C.G. Enke, personal communication). Nevertheless, the mirror parameters made rapidly available by the

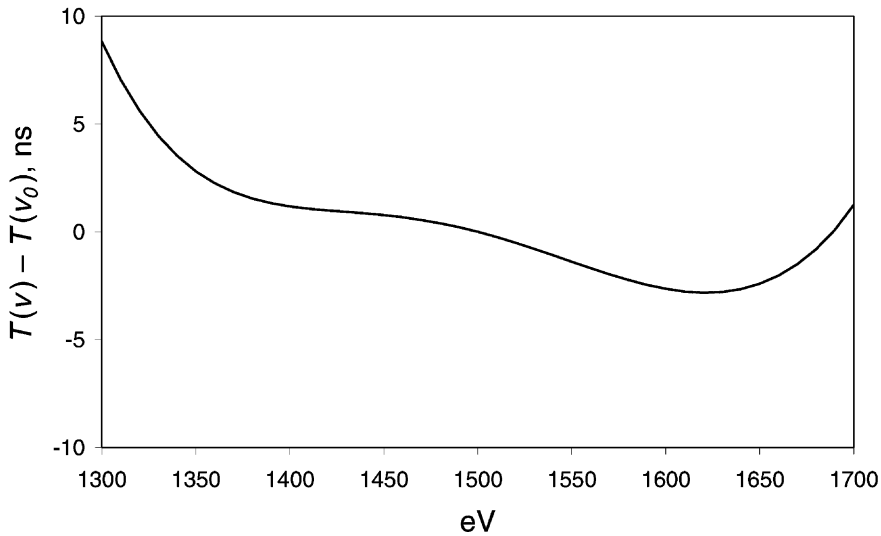

Fig. 6. Flight time deviations for $m/z = 100$ as a function of initial energy for the optimized mirror.

series solution may yield satisfactory focusing, or at least serve as an excellent starting point for enhanced optimization in three dimensions.

3.1. Example

As an example, we consider an instrument with a 1-m field-free flight path, a cylindrical mirror of radius $r = 149$ mm and length $L = 288$ mm, and ion energies between 1300 and 1700 eV, with v_0 corresponding to 1500 eV. Ion mass is arbitrarily chosen to be 100 u. We neglect flight time in the source, thus calculating $T_{\mathrm{ff}}(v)$ as L/v and T_{mirror} from Eq. (13). For the response function, Eq. (14), we choose $n = 4$ and v_i values corresponding to ion energies, in eV, of $\{1350, 1450, 1550, 1650\}$. We set $V_2 \equiv 1.1 \times 1700 = 1870$ V and begin with V_1 at 1300 V, z_1 at $288/4 = 72$ mm and z_2 at $3z_1 = 216$ mm. The following parameters are then found to optimize $F(\boldsymbol{M})$:

$$z_1 = 103\,\mathrm{mm}, \qquad z_2 = 250\,\mathrm{mm}, \qquad V_1 = 1266\,\mathrm{V}$$

Flight time deviations for these parameters are shown in Fig. 6 as a function of initial ion energy.

The flight times fall within a 6-ns range for ions within the optimized energy range (1350–1650 eV). Even better focusing would be expected if flight times in the ion source were considered.

Acknowledgement

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