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CONSTRAINED OPTIMIZATION DESIGN OF AN ION FOCUSING SYSTEM WITH WIDE RANGE OF ENERGY ADJUSTMENT

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Abstract

For the study of ion scattering from solid surface, it is required that the energy of ions can be adjusted widely. The constrained optimization design of an ion focusing system with wide energy range and the magnification less than unity using the improved complex method is proposed in the present paper. This ion focusing system is suitable for use in the low energy ion scattering spectroscopy (ISS) and secondary ion mass spectroscopy(SIMS).

KEY WORDS: Low energy ion focusing system design, Constrained Optimization design, Improved Complex method.

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Introduction

Recently, the ion beam technique is applied widely in these fields: surface analysis in the surface physics such as ion scattering spectroscopy (ISS) and secondary ion mass spectroscopy (SIMS), surface modification in the materials science and microelectronics. For example, an ion optical focusing system with wide adjustable energy range of ions is required for the study of ion scattering from solid surface. Since the design principle of ion optical system is same as that of electron optical system, the general method of computer-aided design (CAD) in electron optics can be used for design of ion optical system, and the low energy electron optical system, especially the main focusing lens, can be used as an ion focusing system. But, there are a few differences between ion focusing and electron focusing: for a given kinetic energy, electrons move more rapidly than ions. Thus ions are less affected by magnetic field than electrons but ions and electrons of a given energy are equally affected by electrostatic field. Therefore electrostatic lenses are generally more efficient at low energy ions than are magnetic lenses[3]. Additionally, in order to avoid the chromatic aberration caused by rotation and fluctuations of the current energizing magnetic field in the magnetic lens, electrostatic lenses, which assemble and adjust easily, are preferable to magnetic lenses in the surface science. In recent years, some ion optical systems are suggested for the surface analytical studies [1-3,6]. However, in these ion optical systems, there are some shortcomings: the number of electrodes is more than or equal to 5 elements, so that the energy of ions is more difficult to adjust widely. The electrostatic lens consisting of four equidiameter cylinders shown in Fig.1 is adopted as an ion focusing lens system. The structure of ion source is based on a Bayard-Alpert ionization gauge. In order to ensure that the spot of ion beam is not greater than the size of aperture of the lens system, it is desirable to keep the magnification M less than unity. The optimum geometric structure and electric parameters of ion focusing lens system designed by using the constrained optimization method is proposed in this paper for the present case. The ion energy range with the magnification M equal to or less than unity can be adjusted conveniently, so it is suitable for use in the low energy scattering spectroscopy (ISS).

Principle and Method

The computer-aided design(CAD) method is often used for the design of electron optical systems. However, there are some limitations in the CAD method: it can only be used to calculate certain electron optical characteristic parameters from given boundary conditions and cannot obtain the practical structure from the electron optical properties directly. The optimization method can determine the final optimum structure of an electron (ion) optical system from given electron (ion) optical properties with criterion of minimum objective functional value (i.e., the spherical aberration coefficient,etc.) directly, so it is good use for the design of the electron (ion) optical systems.

Optimization Method

It is well known that the optimization problem is an extreme value problem of the objective function $f(\vec{x})$ defined in the space of $\vec{x} \in R^n$. The mathematical programming form of constrained optimization problem is:

$$\begin{cases} \min f(\vec{x}) & & \\ x \in R^n & & \\ a_i \leqslant x_i \leqslant b_i & i=1,2,\cdots,n & \text{explicit constraints} \\ g_j(\vec{x}) \leqslant 0 & j=1,2,\cdots,m & \text{implicit constraints} \end{cases} \tag{1}$$

In the present case, the objective function $f(\vec{x})$ is the spherical aberration coefficient $Cs(\vec{x})$; $\vec{x}$ is the search argument vector in the n-dimensional space; the length of electrodes, the gap between two electrodes and the values of electrode potential are taken as components of $\vec{x}$ as well as explicit constraint parameters; the distance IL from the ion source to the image plane and the magnification M may or may not be taken as implicit constraint conditions for the different cases. The point defined in the $\vec{x}$-domain R^n and satisfied with the constraints is called feasible point.

In the common optimization methods, it is necessary to calculate out the objective functional value and the derivative of the objective function with respect to the search arguments, such as the electric parameters and geometric structure parameters of an electron (ion) optical system. Usually, the expression of objective function cannot be written in a closed analytic form of the search arguments, so that the calculation of derivative of the objective function with respect to the search arguments becomes difficult, even impossible. Thus, some methods based on calculation of derivative of objective function (e.g. Gradient Method) are not able to be used for design of electron (ion) optical systems. However, it is not necessary to know the functional relation between the objective function and search arguments and to derive the derivation of the objective function in the Direct Search Method, which needs only to calculate the objective functional value. The Complex Method with constrained conditions[5,7], one of the direct search methods, is better suited than other optimization methods for the design of electron (ion) optical systems.

There are different iterative processes to optimize the objective functional value for the different optimization method. In the complex method, an initial complex should be set up starting with an initial feasible point firstly. Then, the search iteration is carried out, and the optimum point and optimum value of search arguments are found. Because the iterative process of the original complex method contains only two steps: reflection and reduction, so the optimization search rate is not much higher. In order to increase the convergence rate of optimization search process, the original complex method should be improved. The best way is that the two steps, expansion and contraction, are interpolated into the optimization search iterative process. The flow diagram for this improved complex method is shown in Fig.2.

In order to ensure the optimum value point $\vec{x}$ is limited in the feasible-point-set, one should check whether the $\vec{x}$ is a feasible point, if not, readjust $\vec{x}$ to become a feasible point. The method of checking and readjusting feasible points is contained in the improved complex method. In this method, the non-feasible points are readjusted to become feasible points by means of known feasible points. It is the same as the original complex method [5].

Calculation of Electric Field and Electron Optical Properties

The electric field and parameters of electron optical property were calculated, respectively,for each search process in the complex method. The calculation

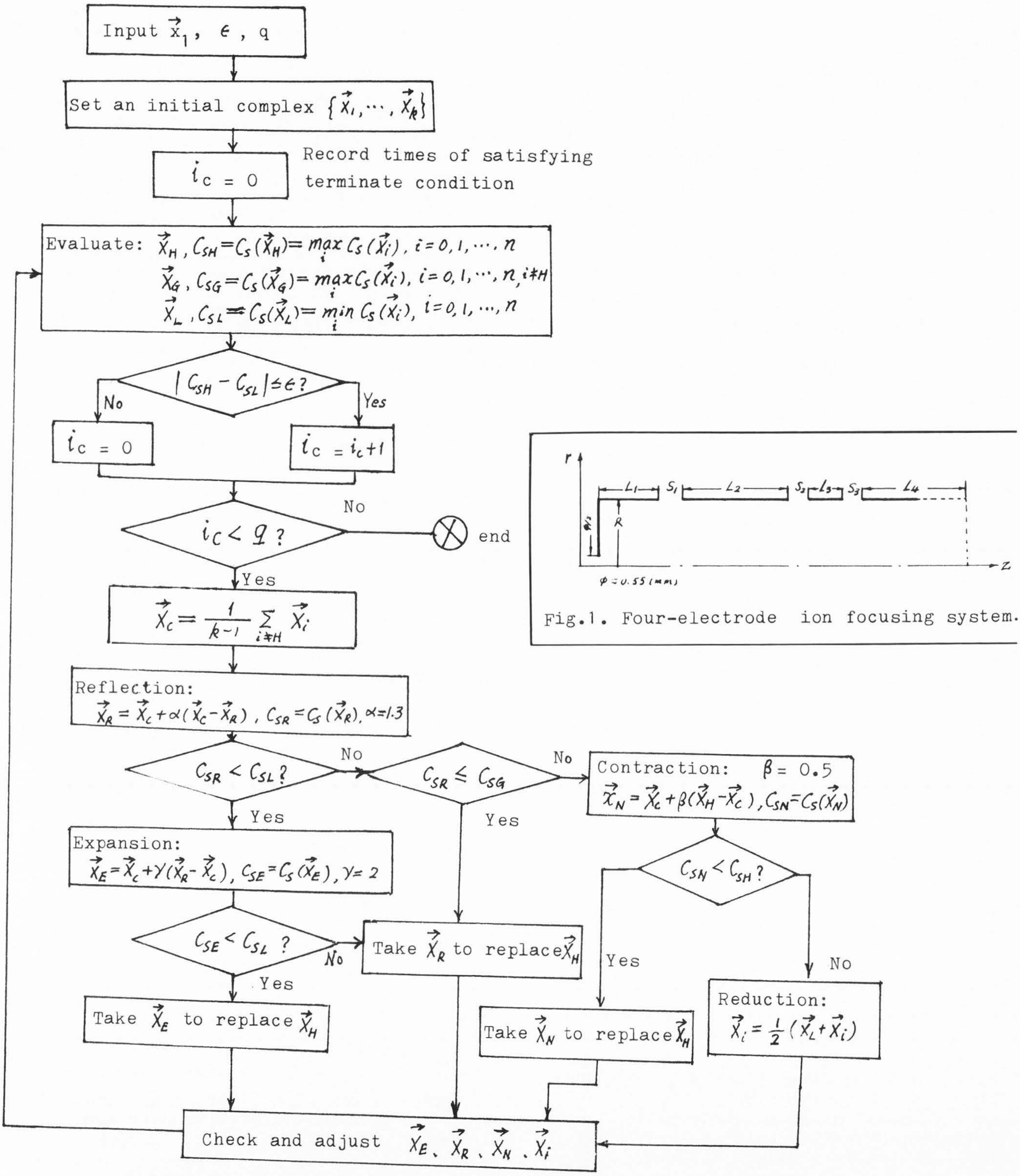

Fig.1. Four-electrode ion focusing system.

Fig.2 : Flow diagram of improved complex method.

method is summarized as follows:

(1) Calculation of electric field.

As we well know, if the ion lens is used as a main focusing system, the space charge effect can be neglected. The evaluation of the electric field in the ion lens shown in Fig.1 will be reduced to a boundary value problem of a rotational symmetrical Laplace equation. The finite difference method with successive overrelaxation is used in the numerical calculation of the Laplace equation. The formulas for calculating the potentials in the lens space are given by:

$$V_{ij}=\left(\frac{1}{a^2}+\frac{1}{b^2}\right)^{-1}\left[\frac{V_{i+1,j}}{2a^2}+\frac{V_{i-1,j}}{2a^2}+\left(1+\frac{b}{2r}\right)\frac{V_{i,j+1}}{2b^2}+\left(1-\frac{b}{2r}\right)\frac{V_{i,j-1}}{2b^2}\right] \quad (r\neq 0) \qquad (2)$$

$$V_{ij}=\left(\frac{1}{a^2}+\frac{2}{b^2}\right)^{-1}\left[\frac{V_{i+1,j}}{2a^2}+\frac{V_{i-1,j}}{2a^2}+\frac{2V_{i,j+1}}{b^2}\right] \quad (r=0) \qquad (3)$$

where a, b are the axial and radial steps of rectangle mesh, respectively; r is the distance from the axis to the mesh nodal point.

The residual error in the overrelaxation iteration is defined as follows:

$$V_w^{(k+1)}-V^{(k)}=w\left[V^{(k+1)}-V^{(k)}\right] \qquad (4)$$

where k is number of the iterative times and w is overrelaxation factor, generally $1\leq w\leq 2$. The selection of w value, which depends on the number of mesh nodal points and the iterative calculation order, is the key to the rate of convergence. In our calculation of electric field, w=1.8 was used for 50 times for initial iteration, then the new value of w is chosen as:

$$W_1=W_0+0.1\times(2-W_0) \qquad (5)$$

where

$$W_0=1+\frac{\lambda}{(1+\sqrt{1-\lambda})^2} \qquad (6)$$

and λ is defined by

$$\lambda=\sqrt{\frac{\sum_i\left[V_i^{(50)}-V_i^{(49)}\right]}{\sum_i\left[V_i^{(49)}-V_i^{(48)}\right]}} \qquad (7)$$

where $V_i^{(48)}$, $V_i^{(49)}$, $V_i^{(50)}$ are potential values of i^{th} node in the 48^{th}, 49^{th}, 50^{th} iteration, respectively.

When the residual error in the calculation of electric field is less than 10^{-8}, the calculation is stopped.

(2) Calculation of electron optical parameters.

The well-known Scherzer formula is used for the calculation of the spherical aberration coefficient.

$$C_s=\frac{1}{16\sqrt{\Phi_0}}\int_{z_0}^{z_n}\phi^{-3/2}\left[\frac{5}{4}\phi''+\frac{5}{24}\cdot\frac{\phi'^4}{\phi^2}+\frac{14}{3}\frac{\phi'^3}{\phi}\frac{r_1'}{r_1}-\frac{3}{2}\phi'^2\left(\frac{r_1'}{r_1}\right)^2\right]\cdot r_1^4\,dz \qquad (8)$$

where r_1 is a paraxial-ray emitted from the object point on the z axis with 45° initial emission angle, Φ_0 is the potential at the object point, ϕ' and ϕ'' are first and second derivatives of the axial potential with respect to z, respectively, z_0 is the object plane position, z_n is the image plane position.

The electron optical characteristic parameters: principal point, focal point and focal length are determined in the usual way.

The calculation of the electron trajectory makes use of the Picht equation:

$$\rho''+\frac{3}{16}\left(\frac{\phi'}{\phi}\right)^2\cdot\rho=0 \qquad (9)$$

where $\rho=r\cdot\phi^{1/4}$

The Fox-Goodwin formula shown as follows is used for the numerical calculation of the Picht equation.

$$\left(1-\frac{1}{12}a^2g_{i+1}\right)\rho_{i+1}=\left(2-\frac{5}{6}a^2g_i\right)\rho_i-\left(1-\frac{1}{12}a^2g_{i-1}\right)\rho_{i-1} \qquad (10)$$

where

$$g_i=-\frac{3}{16}\left(\frac{\phi_i'}{\phi_i}\right)^2;\quad \phi_i'=\frac{\phi_{i+1}-\phi_{i-1}}{2a} \qquad (11)$$

and a is an axial step.

Computed Results and Discussion

Computed Results

The optimization design of an ion optical system described in this paper is divided into two parts as follows.

(1) Part 1: Searching optimum values with fixed ion energy.

In this case, the ion beam energy is adjusted through varying the values of electrode potential in the same proportion. The implicit constraints are:

$$\begin{cases}100.0-IL(\vec{x})\leq 0.0\\ M(\vec{x})-1.0\leq 0.0\end{cases}$$

and the search arguments are constrained. The explicit constraints are:

$4.0\leq L3\leq 6.0$ (mm),
$1.2\leq S1\leq 1.5$ (mm),
$50\leq V2\leq 90$ (v).

The adjustment ranges of feasible points of L3, S1, and V2 are given by:

$\delta_1=0.5$mm, $\delta_2=0.5$mm, $\delta_3=10$v

The typical computed results are listed in Table 1.

Table 1. The typical computed results.
Fixed parameter: R=4.5, L1=5.0, L2=15.2, L4=15.0, S2=S3=1.5(mm), V1=20, V3=90, V4=350(v).

No	Ion Energy (ev)	L3 (mm)	S1 (mm)	V2 v	IL (mm)	M	Cs
1	350	5.0	1.5	70	111.9	1.0	160.4
2	350	4.5	1.5	70	108.9	0.99	153.5
3	350	4.5	1.5	60	102.9	0.92	158.3
4	350	4.5	1.3	70	110.6	1.0	147.5

(2) Part 2: Change ion energy, searching for optimum values.

In this part, the implicit constraint is only image plane location and the search parameters are not constrained. The ion energy is adjusted by means of varying the ratio V3/V4 and value of V4. The implicit constraint is:

$$105.5 \leqslant IL(\vec{x}) \leqslant 110.5$$

The main computed results are as listed in Table 2.

The variable-focusing voltage V3 vs eV4 (ion output energy) is shown in Fig.3. There are two voltage modes, low mode ($V3 < V4$) and high mode ($V3 > V4$), for the curve of V3 vs eV4. The magnification M vs eV4 is shown in Fig.4.

Table 2. The main computed results in part 2.
Fixed Parameters: R=4.5, L1=5.0, L2=20.0, L3=8.5, L4=13.0(mm), S1=S2=S3=1.5(mm), V1=20, V2=100(v)

Mode	Ion energy: eV	V3 (v)	IL (mm)	M	Cs
Low $V_3 < V_4$	22	20	106.9	2.69	237.1
	40	20.5	109.7	2.33	351.0
	100	28	106.5	1.59	465.2
	320	68	108.4	1.08	325.6
	500	110	106.7	0.94	206.3
	650	155	107.2	0.93	121.3
	792	440	105.6	1.12	66.5
	800	230	106.7	0.92	84.8
High $V_3 > V_4$	12	30	107.6	2.77	221.1
	12.1	40	108.6	2.57	362.0
	22	100	109.5	1.95	618.8
	40	175	107.7	1.70	412.7
	100	322	110.4	1.68	153.0
	300	490	107.8	1.53	80.1
	500	513	106.6	1.38	73.0

The constraint condition: IL=108.0±2.5(mm)

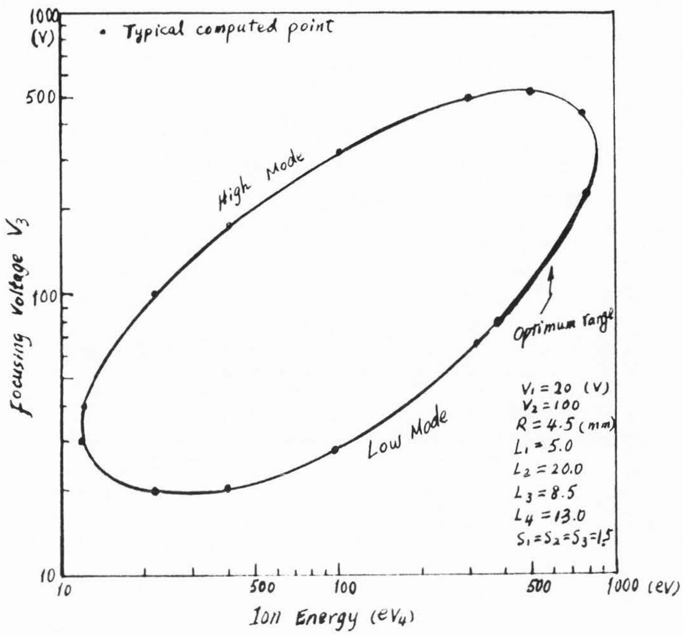

Fig.3. Variable-focusing voltage V3 vs ion energy (eV_4).

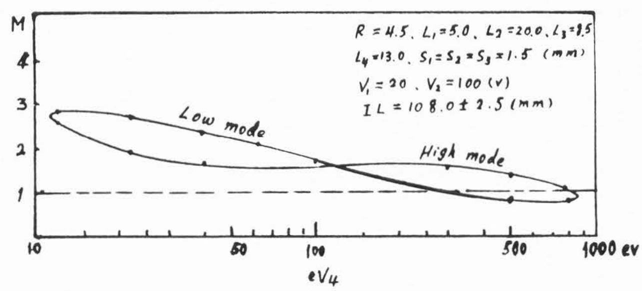

Fig.4. Magnification M vs ion energy (eV4).

Discussion

In part 1, from Table 1, it is seen that No.4 data is a data of best point which magnification is equal to unity. When the values of electrode potential is varied in the same proportion to adjust the ion energy, the electron optical properties cannot be changed.

In part 2, from Fig.3, we can know that the ion energy can be variated from 420 to 890 eV while magnification M is less than unity and the image location is from 105.5mm to 110.5mm. If the magnification M is not critical, the energy of ion beam can be adjusted from 10 to about 1000 eV while the position of image plane is nearly fixed. Therefore, this ion lens system with an aperture stop positioned at the entrance and exit, in which the beam spot at image plane can be kept constant, may be suitable for use in the ion analysis technique.

The Simplex Method is another direct search method in the optimization problem [4], but there are no constraint conditions in it, so there must be an on-line control of search parameters to satisfy the desired requirements during the optimization process. This makes automatic search difficult. Hence, although the simplex method is a usable method for electron (ion) optical system design, it still suffers some shortcomings. Therefore, the complex method is better than the simplex method in the design of electron (ion) optical systems.

The corresponding electron (ion) optical transfer function (OTF) of the ion optical system is also calculated. The OTF is defined by:

$$OTF = M_i(f)/M_o(f) \qquad (12)$$

where $M_o(f)$ and $M_i(f)$ are frequency spectra in the object space and the image space of ion beam, i.e., the Fourier transform of distribution function of the object and image, respectively.

The ion optical system designed by the improved complex method described above has some advantages: simple geometric structure and easy to adjust the ion energy, so it is better suited for use in low energy ion scattering spectroscopy ISS and SIMS.

If the current of ion beam with a given spot size at image plane is taken as the search objective function, the optimization program would be modified to find the optimum magnification or arrangement both of the electrodes and the magnification. It may be possible to find other structures.

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Discussion with Reviewers

T. Mulvey: Would you agree that magnetic lenses with their lower aberrations are however not suitable for ion beam focusing? Do you agree that the principal problem with ion sources is the chromatic aberration rather than spherical aberration?

Authors: Since electrons move more rapidly than ions for a given kinetic energy, ions of a given energy are less affected by magnetic field but ions and electrons are equally affected by electrostatic fields. Therefore, although the chromatic aberration of magnetic lenses is lower than that of electrostatic lenses, the electrostatic lenses are generally more efficient at focussing low energy ions than are magnetic lenses.

T. Mulvey: If you consider sources which have a large effective source size, the optimising program may have to be altered to allow for this to be taken into account. Could you supply more information on this point?

Authors: It is possible. Our optimization method can satisfy different desired requirements. Of course, the optimizing program may have to be altered, i.e., the objective function or constrained conditions in the optimization method should be changed to allow for the different design parameters (e.g., different effective ion source size, etc.).

T. Mulvey: Have you any evidence to support the view that the magnification of the system is about unity or even less? The programe could be asked to find the optimum magnification to achieve that the current could be delivered into a spot of given diameter in the image plane?

Authors: In our case, the structure of ion source with aperture at extractor is based on the Bayard-Alpert ionization gauge, the design requirement is that the spot size in the image plane is not greater than the diameter of the extractor aperture, so that the magnification $M \leq 1$ is desired.

If the current of ion beam with a given spot size at image plane is taken as an objective function, the programe may be altered to find other structures of ion focusing system with an optimum magnification or arrangement both of the electrodes and the magnification.