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CONSTRAINED OPTIMIZATION DESIGN OF AN ELECTRON OPTICAL SYSTEM

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Abstract

An electron optical system can be optimized using the "simplex method" or "complex method". By these methods, the final structure of an electron optical system, for example, an extended field lens (EFL), can be searched with a criterion of minimum objective parameter (in the present case, the coefficient of spherical aberration). Because there is no constraint in the simplex method, the constrained optimization method (the complex method) described in this paper is better than the simplex method in the design of electron optical systems. In the simplex method as well as the complex method, it is not necessary to know the explicit functional relation between the objective function and the searching parameters; and the variations of aberration coefficient with respect to some machining tolerance can be easily obtained. Therefore, comparing with other optimization methods, the simplex method and complex method have significant advantage in the optimization design of electron optical systems.

KEY WORDS: Electron optical system design, Constrained optimization design, Complex method.

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Introduction

The computer-aided design (CAD) method for electron optical systems has been considerably developed since the 1960's. However, there are some limitations in the application of the CAD method in electron optical systems; this CAD method can only be used to calculate certain electron optics characteristic parameters from given boundary conditions, such as geometric structure and electrical parameters[2]. In recent years, the question of how to determine the optimal structure and the corresponding electrical parameters of an electron optical system from given electron optics characteristic parameters, i.e. the optimization design of electron optical systems, has gradually received more attention.

The optimization design method is a method which can minimize the objective function (e.g. an aberration coefficient of the electron optical system) under certain constraint conditions, from which the optimal structure can be obtained. In this method, some suitable geometric and electrical parameters are chosen as the search parameters.

The optimization design is an objective which has been sought by electron optics researchers for a long time. Some optimization design methods[5,6,8-11] for electron optical systems have been suggested since the 1970's. Using the dynamical programming method of Szilagyi[9-11] and the variational method of Rose[8], the potential and/or magnetic field distribution along the electron optical system's symmetry axis producing a minimum spherical aberration could be searched. However, the final optimal structure cannot be obtained by these methods. In order to determine the optimal structure, it is necessary to carry out experimental analog studies conforming with the potential distribution along the symmetry axis obtained by these methods. The "Simplex Method", an optimization design method in electron optics as suggested by Gu and Chen[1] in 1982, can overcome the disadvantages of both the dynamical programming and the variational methods. The optimal structure can be directly obtained with a criterion of minimum spherical aberration coefficient using the simplex method. However, there are no constraint conditions in the simplex method, so there must be an on-line control of the search parameters during the optimization process. This makes automatic search difficult. Hence, although the simplex method is a usable method for electron optical system design, it still suffers some shortcomings.

The "Complex Method" proposed in this paper is an important improvement in the optimization design method of electron optical systems.[7] It is a multidimensional "constrained-extreme-value problem". Not only can the optimal structure be searched and corresponding parameters be obtained automatically, but one can also be certain that the results will satisfy the constraint conditions.

Principle

In the optimization design of electron optical systems, the electron optics characteristic parameters are chosen as the optimization objective function (or "error function"). It is defined as the sum of weighted squares (or the square root of the sum of weighted squares) of various electron optical aberration coefficients. Some of the aberration coefficients $f_1, f_2, \ldots, f_m$ (e.g. spherical aberration, central chromatic aberration, axial astigmatism, etc.) will be used as components of the objective function subject to the concrete requirements. Each kind of aberration coefficient $f_i (i=1,2,\ldots,m)$ is regarded as a function of certain geometric parameters (e.g., the diameter or length of an electrode cylinder, the gap between two electrodes, the shape of the magnetic pole pieces, etc.) and electrical parameters (e.g. the electrode potentials, the currents driving the magnetic field, etc.). These parameters will be taken as the search parameters expressed as $x_1, x_2, \ldots, x_n$. Thus, the objective function is defined as follows:

$$f(\vec{x}) = \sum_{i=1}^{m} (W_i f_i(\vec{x}))^2 \tag{1}$$

or

$$f(\vec{x}) = [\sum_{i=1}^{m} (W_i f_i(\vec{x}))^2]^{\frac{1}{2}} \tag{2}$$

where $\vec{x}$ is an independent vector-argument in the n-dimensional space:

$$\vec{x} = (x_1, x_2, \ldots, x_n)^T \tag{3}$$

where T refers to transposition and $x_1, x_2, \ldots, x_n$ are n unknown search arguments. The $\vec{x}$-domain is R^n. Each W_i is a weighted factor, $0 < W_i \le 1$, $i=1,2,\ldots,m$, determined according to the design requirements.

Mathematically, the optimization problem is an extreme value problem of the objective function $f(\vec{x})$ defined in the space of $\vec{x} \in R^n$. Its mathematical programming form is:

$$\begin{cases} \min\limits_{\vec{x} \in R^n} f(\vec{x}) & (4) \\ a_i \le x_i \le b_i \quad i=1,2,\ldots,n & \text{explicit constraints} \\ g_j(\vec{x}) \le 0 \quad j=n+1,\ldots,m & \text{implicit constraints} \end{cases}$$

This problem is a nonlinear programming problem.

In the design of electron optical systems, the limitation on a part of the search parameters, e.g., the size of an electrode cylinder and magnetic pole, the values of electrode potential and driving current etc., will be taken as the explicit constraint conditions. The limitation on the electron optical characteristic parameters, which are implicit functions of the search arguments, can be taken as the implicit constraint conditions. As it is known, the spherical aberration coefficient can be used as a criterion for the performance of an electron lens under a fixed focal length condition. However, the focal length of the lens is an implicit function of the search arguments. Usually, the expression of the functional relations between the focal length and the search arguments cannot be written in a closed form. Only if the iterative calculation of the potential or the magnetic field is finished, the focal length of the lens can be evaluated in accordance with a certain geometrical structure and electrical parameters. Therefore, the limitation on the focal length can be taken as an implicit constraint condition in the optimization design of electron optical systems.

The complex method described in this paper is used as a constrained optimization design method of electron optical systems, i.e., an electron optics constrained extreme value problem. The complex used in this method is a polyhedron which has k vertices in the n-dimensional space: $\{\vec{x}(1), \vec{x}(2), \ldots, \vec{x}(k)\}$, $k \ge n+2$, usually we take $k=2n$. In order to avoid degeneracy, k should be taken at a high value.

The complex method is summarized as follows:

A. The complex method iterative process:

(i) Give an initial feasible point $\vec{x}^{(1)}$. Feasible means that this point is defined in the $\vec{x}$-domain and satisfies the constraint conditions.

(ii) Starting with $\vec{x}^{(1)}$, set up an initial complex $\{\vec{x}^{(1)}, \vec{x}^{(2)}, \ldots \vec{x}^{(k)}\}$. The vertices of the complex must be limited in the feasible set.

(iii) Calculate the worst point $\vec{x}^{(h)}$ and the best point $\vec{x}^{(\ell)}$ among the vertices of the complex, i.e. the point of maximum and minimum value of $f(\vec{x})$:

$$f(\vec{x}^{(h)}) = \max_i f(\vec{x}^{(i)}) \tag{5}$$

$$f(\vec{x}^{(\ell)}) = \min_i f(\vec{x}^{(i)}) \tag{6}$$

(iv) Calculate $\bar{x}$ - the centroid of the complex excluding $\vec{x}^{(h)}$, i.e. calculate the vectorial mean:

$$\bar{x} = \frac{1}{k-1} \sum_{i \ne h}^{k} \vec{x}^{(i)} \tag{7}$$

(v) Calculate $\vec{x}^{(r)}$ - the reflection point of $\vec{x}^{(h)}$ with respect to $\bar{x}$, i.e.

$$\vec{x}^{(r)} = \bar{x} + \alpha(\bar{x} - \vec{x}^{(h)}) \tag{8}$$

where $\alpha>1$; generally, $\alpha = 1.3$.

(vi) Check whether the $\vec{x}^{(r)}$ is a feasible point, if not, readjust $\vec{x}^{(r)}$ to become a feasible point.

(vii) Take $\vec{x}^{(r)}$ instead of $\vec{x}^{(h)}$, if it cannot improve the worst point position, $\vec{x}^{(r)}$ should be constricted towards $\bar{x}$ until it satisfies the requirement.

The terminate condition of the complex method is

$$f(\vec{x}^{(h)}) - f(\vec{x}^{(\ell)}) \leq \varepsilon \, . \qquad (9)$$

The condition (9) should be satisfied q times consecutively, where ε is the accuracy the objective function is to be computed with.

The complex method calculation flow diagram is shown in Fig. 1.

B. The method of checking and readjusting the feasible points

In this method, the non-feasible points are readjusted to become feasible points by means of known feasible points: $\vec{d}^{(1)}, \vec{d}^{(2)}, \ldots, \vec{d}^{(s)}$. This process is shown as follows:

(i) If $\vec{x}$ cannot satisfy the explicit constraints, it should be adjusted with a small displacement δ_i such that

$$\text{if } x_i > b_i, \text{ then } x_i = b_i - \delta_i \; ;$$

$$\text{if } x_i < a_i, \text{ then } x_i = a_i + \delta_i \; ;$$

the value of δ_i depends on practical requirements of the electron optical systems.

(ii) If $\vec{x}$ cannot satisfy the implicit constraints, it should be constricted towards the centroid of the set of points $\vec{d}^{(1)}, \vec{d}^{(2)}, \ldots, \vec{d}^{(s)}$:

$$\vec{x}^{(N)} = \frac{\vec{x} + \vec{x}^{(c)}}{2} \qquad (10)$$

where

$$\vec{x}^{(c)} = \frac{1}{S} \sum_{i=1}^{S} \vec{d}^{(i)} \; . \qquad (11)$$

(iii) Repeat step (i) and recheck if $\vec{x}$ satisfies the explicit and implicit constraints until $\vec{x}$ is a feasible point.

The flow diagram for this method is shown in Fig. 2.

An Example and Results

An Extended Field Lens (EFL) is taken as an example for optimization design using the complex method. The computed results for EFL using the CAD and simplex method have already been obtained before.[1,3,4] The 4EFL structure (it consists of 4 equidiameter electrodes) is shown in Fig. 3.

In this paper, the spherical aberration is taken as an objective function, the length and potential of electrodes, and the gap between the electrodes are taken as the search arguments.

Owing to the limitation of computer capacity at our university, the method of successive optimal search in two dimensional space is used

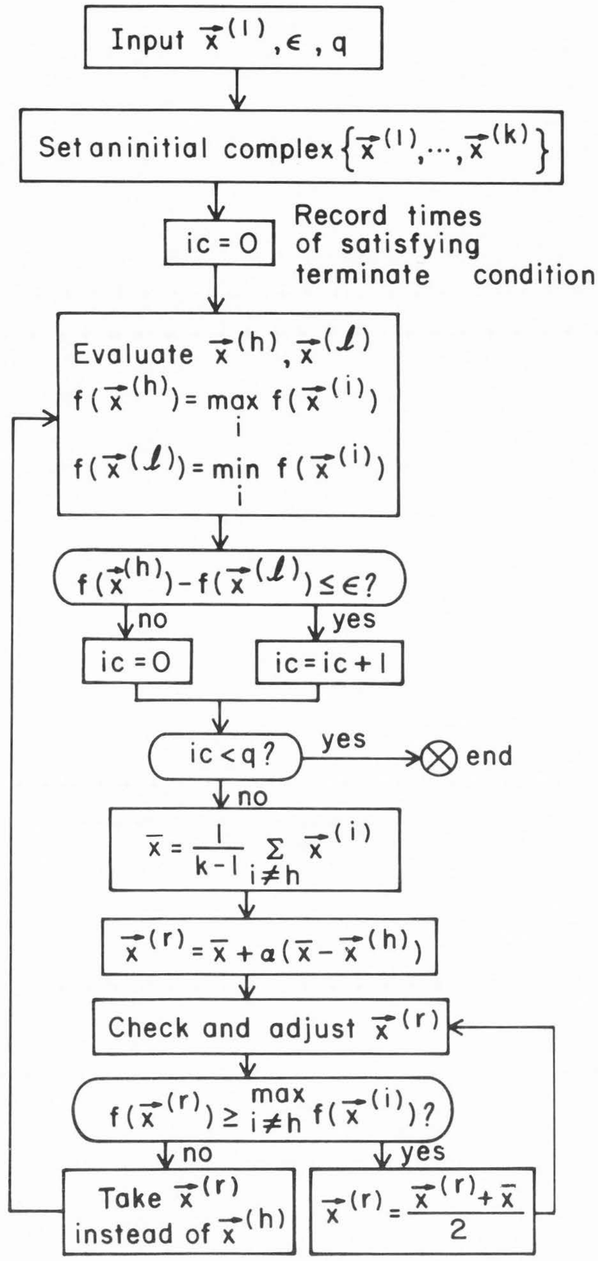

Fig. 1. Flow diagram for the complex method.

in the present case. We change the pair of search arguments: $L_3, S_3; L_2, L_3$ and V_2, V_3 respectively in each searching process.

The explicit constraints are

$$\begin{array}{llll} 15.0 \leq L_2 \leq 25.0 & \text{(mm)} \\ 1.0 \leq L_3 \leq 5.0 & \text{(mm)} \\ 1.0 \leq S_3 \leq 3.0 & \text{(mm)} & & (12) \\ 6.0 \leq V_2 \leq 8.0 & \text{(kV)} \\ 9.0 \leq V_3 \leq 12.0 & \text{(kV)} \end{array}$$

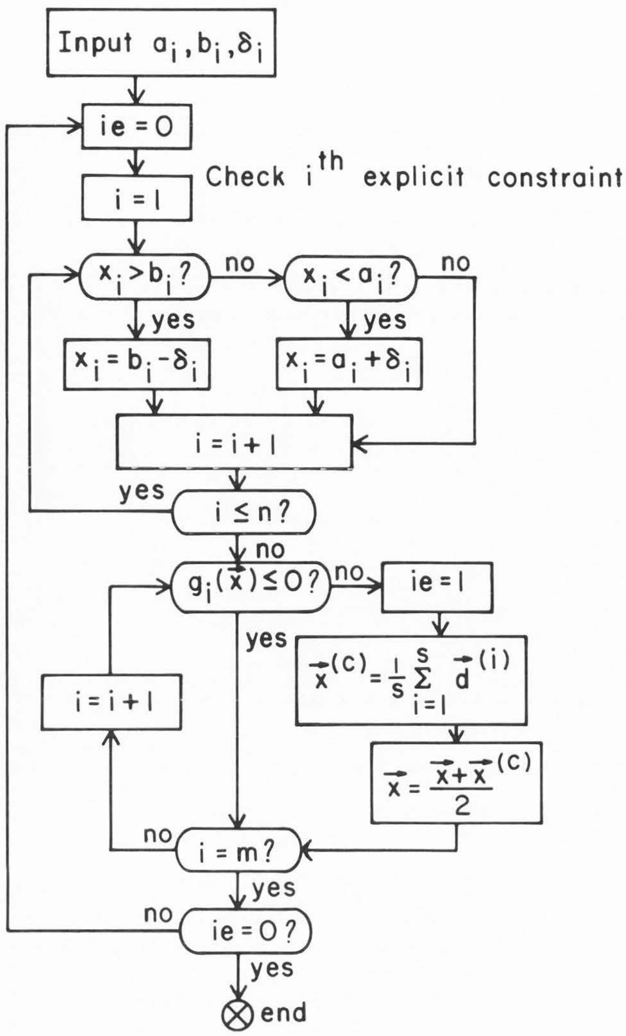

Fig. 2. Flow diagram for checking and adjusting the feasible point.

The implicit constraint is

$$F_2(\vec{x}) - 50.5 \leq 0 \;, \qquad 13)$$

where F_2 is the image space focal length.
Let ε = 0.5, $\delta_1 = \delta_2 = \delta_3 =$ 0.5 (mm), $\delta_4 = \delta_5 =$ 0.2 kV.

Because the 4EFL is often used as a main lens in electron optical systems, the potential on the electrodes and the electron velocity in the space of 4EFL are rather high. Therefore, the space charge effect can be neglected. The evaluation of the electric field in the space of 4EFL can be reduced to a boundary value problem of a rotational symmetrical Laplace equation.

The finite difference method with successive overrelaxation was used in the numerical calculation of the Laplace equation. The selected value of relaxation factor ω depends on the number of mesh nodal points and the iterative calculation order. For some optimum value ω between 1 and 2, the rate of

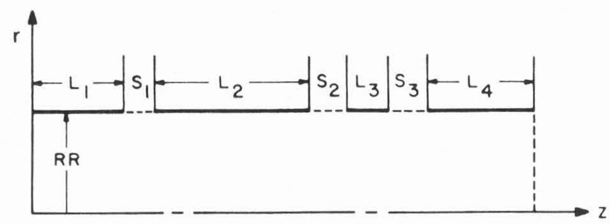

Fig. 3. 4EFL (Extended Field Lens) structure.

convergence can be improved. The auto-selected value of the ω factor is used in our calculations.

The famous Scherzer formula is used for the calculation of the spherical aberration coefficient.

$$C_s = \frac{1}{16\sqrt{\phi_0}} \int_{z_0}^{z_n} \phi^{-3/2} \left[\frac{5}{4}\phi''^2 + \frac{5}{24}\frac{\phi'^4}{\phi^2} + \frac{14}{3}\frac{\phi'^3}{\phi}\cdot\frac{r_1'}{r_1} - \frac{3}{2}\phi'^2\left(\frac{r_1'}{r_1}\right)^2\right] r_1^4 \, dz \qquad (14)$$

where $z = z_0$ is the objective plane, $z = z_n$ is the image plane, r_1 is a paraxial-ray emitted from the objective point on the axis with 45^0 initial emission angle, ϕ_0 is the potential at the objective point, ϕ' and ϕ'' are first and second derivatives of the axial potential with respect to z respectively.

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

$$\rho'' + \frac{3}{16}\left(\frac{\phi'}{\phi}\right)^2 \rho = 0 \;, \qquad (15)$$

where

$$\rho = r\,\phi^{1/4} \,.$$

The method of the parallel trajectory is used for computing the electron optical characteristic parameters: principal point, focal point and focal length.

The Fox-Goodwin formula shown as follows is used for the numerical calculation of Eq. (15)

$$\left(1 - \frac{1}{12}a^2 g_{n+1}\right)\rho_{n+1} = \left(2 + \frac{5}{6}a^2 g_n\right)\rho_n - \left(1 - \frac{1}{12}a^2 g_{n-1}\right)\rho_{n-1}$$

where

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

and a is an axial step. The results computed using the CAD method are used to form the initial complex.

The computed results using the complex method are listed in Table 1. For the purpose of comparison, the computed results using the simplex method and the CAD method are also shown in this table.

Table 1. The Main Computed Results

Fixed Parameters: RR = 4.5 mm L_1 = 13.0 mm S_1 = 2.0 mm S_2 = 2.0 mm L_4 = 13.0 mm V_4 = 30 kV

Method	No	L_2 mm	L_3 mm	S_3 mm	V_1 kV	V_2 kV	V_3 kV	F_2 mm	C_s	Remarks
Complex	1	20.0	4.00	3.00	10.0	7.0	10.0	50.11	763.2	The initial complex
	2	"	4.26	2.50	"	"	"	50.35	795.9	L_3,S_3 searching process
	3	"	2.86	2.50	"	"	"	46.41	802.0	"
	4	"	3.36	2.94	"	"	"	48.77	728.5	L_3,S_3 optimal point
	5	20.0	3.50	2.94	"	"	"	48.81	734.1	L_3,L_2 initial value
	6	15.5	2.943	2.938	"	"	"	47.75	457.2	L_3,L_2 optimal point
	7	15.5	2.943	2.938	10.0	6.0	11.0	41.39	408.6	V_2,V_3 initial value
	8	15.5	2.94	2.94	10.0	6.9	11.8	50.10	371.9	V_2,V_3 optimal point
Simplex	9	20.0	4.00	3.00	10.0	7.0	10.0	50.11	763.2	L_3,S_3 initial value
	10	"	3.54	2.80	"	"	"	48.78	730.4	L_3,S_3 optimal point
	11	"	2.56	4.60	"	"	"	49.72	664.7	S_3 too large
	12	16.5	4.24	2.80	"	"	"	49.90	549.9	L_3,L_2 initial value
	13	16.5	4.00	2.80	"	"	"	49.81	541.8	L_3,L_2 optimal point V_2,V_3 initial value
	14	"	"	"	"	5.85	11.3	40.76	393.2	V_2,V_3 optimal point
CAD	15	20.0	4.0	3.2	10.0	7.0	10.0	50.61	826.9	CAD optimal result
	16	14.5	9.5	2.0	8.0	6.0	8.0	46.94	1152.5	" worst result

Discussion and Conclusions

A. From the computed results listed in Table 1, it can be seen that the computed results using the complex method are consistent with the computed results using the simplex method; and the former are better than the latter. Using the complex method, the relative value of the coefficient of spherical aberration decreases from 826.9 to 371.9 while maintaining the same focal length.

B. The computed results using the simplex method show that the spherical aberration coefficient C_S reduces as the gap S_3 increases (see No. 11 in Table 1). Of course, this is consistent with the electron optics principle: the distribution of potential along the axis is extended as the gap S_3 increases. This consequence is beneficial to the reduction of the spherical aberration coefficient. But, if the gap S_3 is too large, the external electric and magnetic field will interfere with the electric field in the lens, and the image focal length will increase, and the design requirement cannot be satisfied. Since there are no explicit and implicit constraints in the simplex method, the aforementioned consequence is hard to avoid. However, using the complex method there is no such situation, so the constrained optimization design method (the complex method) is better than the simplex method in the design of electron optical systems.

C. In the complex method as well as simplex method, variations of C_S, the spherical aberration coefficient, caused by small changes of the search parameters due to machining tolerances are readily available from the computed data in the search process. It is quite accurate and easy to obtain in comparison with the calculation of the spherical aberration coefficient by using theoretical aberration coefficient formulas.

D. In this paper, the computed results show that the choice of the search arguments, the calculation of the objective function and the determination of the constraints are reasonable. In the simplex method and the complex method, it is not necessary to know the explicit functional relation between the objective function and the searching parameters; and the variations of aberration coefficients with respect to some machining tolerance can be easily obtained. Therefore, comparing with other optimization methods, the simplex method and complex method have significant advantage in the optimization design of electron optical systems. The complex method provides an effective mathematical method for the optimization design of electron optical systems. This method has a wide-range application in the field of high resolution electron beam technique.

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