COMPUTER-AIDED DESIGN
OF AXISYMMETRIC ELECTROSTATIC LENSES*

A. HAVAS, A. SÓLYOM, G. HÁRS and L. BORI

Department of Atomic Physics
Technical University H-1521, Budapest

Abstract

A CAD system named *GUNSMITH* is developed to design axisymmetric electrostatic lenses. The system runs on any IBM compatible computer with CGA graphic card, 640 kbyte of main memory, two floppy disc drives or one floppy drive and one hard disc drive, though an AT with a math coprocessor chip is recommended. It can calculate the most important properties of a charged particle optic, namely:
— the axial and the radial potential function,
— the first order optical properties,
— the transfer matrix and its derivates,
— the magnification,
— the chromatic aberration and
— the particle density of the beam as well
within a reasonably short time. Using the system described here the engineer can compare the effects of different electrode shapes without the expense of building an actual optical system. To test the *GUNSMITH* we have calculated the properties of some electrostatic lenses, and the results agree very well with the literature and with the experiments. For example the *GUNSMITH* was used to calculate the parameters of a SIMS ion gun, and the comparisons with the measurements also show fair agreement.

I. Introduction

There are a variety of CAD programs capable of calculating the properties of a charged particle optic [8], [9]. Unfortunately these CAD programs usually require a mainframe computer and a lot of main memory. As now there is a personal microcomputer on every engineer's desk it is natural that a particle optic designer CAD package had to be developed for microcomputers. With this in mind we developed the interactive, menu driven *GUNSMITH* program system for microcomputers. With it is now cost-effective and comfortable to calculate the optical properties of a beam transport system without building it. This CAD system includes a program library and a data base. (The detailed description of the system is given in part III.) A comfortable pull-down menu links all the programs in the library. The results of the calculations are put into the database for future references.

* Dedicated to Prof. J. Giber on the occasion of his 60th birthday.

Using the data in the data base it is possible to combine single or compound lenses to create (other) compound electrostatic optical systems and long beam transport systems. Of course the user can define new types of simple lenses as well i.e. can expand the assortment of the elements. Section II of this paper describes the computer model applied in our system. In section III the most important properties and the usage of this system are described. Finally section IV contains some examples of the capability of the system and results obtained with it. These results are compared with measurements on corresponding optical systems or with the literature.

II. The computer model of the CAD system

Our CAD system can calculate the optical properties of an axisymmetric particle optic containing an arbitrary number of electrodes all of which can have a shape of a cylinder, of a disc or of a cone. It deals with space charge free systems in the non-relativistic limit and in the paraxial ray approximation [1]. The ρ electrostatic potential of a space charge free electrostatic optical system is the solution of the

$$\Delta\rho = 0 \tag{1}$$

Laplace — equation, where the ρ potential is given on the boundaries. (If we did not neglect the space charge we would have to deal with the Poisson — equation instead.) The charge density method [2], [4] has been used to solve this equation. (The advantages of this method over the generally used finite element method [3], [8], [9] are first that it can be applied for infinite systems too and secondly that it requires less memory.) In this method the Laplace equation is transformed into the integral equation:

$$\frac{1}{\pi\varepsilon_0} \int\limits_{L_k} \frac{\sigma(r,z)r}{[(r+r_i)^2+(z-z_i)^2]^{1/2}} K(k(r_i,z_i))dl = \rho(r_i,z_i) \tag{2}$$

where σ is the unknown charge density distribution at the surface of the electrodes, L_k is the contour line of the electrodes in the $r-z$ cylindrical coordinate system (r_i, z_i) an arbitrary point on the L_k contour, $\rho(r,z)$ is the known potential function of the electrodes and dl is the arc length of the L_k contour,

$$k(r_i,z_i) = \left[\frac{4rr_i}{(r+r_i)^2+(z-z_i)^2} \right]^{1/2} \tag{3}$$

and $K(k)$ is the complete elliptic integral of the first kind [7]. The (2) integral equation is used to determine the charge densities. To find an approximate solution we have written the unknown σ charge density function as a linear

combination of stepwise constant $[\phi_i]_{i=1}^\infty$ base functions [5]. Equation (2) then becomes a matrix equation:

$$\mathbf{K}\sigma = \rho \tag{4}$$

where the $K_{i,j}$ matrix element is the potential of the i-th curve element, provided that the charge density on the j-th element is unity and the charge density on the other elements are zero:

$$K_{i,j} = \frac{1}{\pi\varepsilon_0} \int\limits_{l_j - \Delta l_j}^{l_j + \Delta l_j} \frac{r}{[(r+r_i)^2 + (z-z_i)^2]^{1/2}} K(k) dl \tag{5}$$

The charge density distributions are computed using Gaussian elimination [6]. These charge density distributions are used to calculate the axial and radial potential distributions, from equation (2). With the known Φ axial potential distribution the

$$\frac{d^2 r}{dz^2} + \frac{\Phi'}{2\Phi} \frac{dr}{dz} + \frac{\Phi''}{4\Phi} r = 0 \tag{6}$$

paraxial ray equation is solved to obtain the trajectories of sample particles. Equation (6) is integrated with the fourth order Runge-Kutta method. Using this ray equation the transfer matrix can be expressed in a very simple way. Let us designate by r_1 the distance of the sample particle from the lens axis at the exit plane, and by r_1' the slope of the trajectory at the same place. In this case r_1 and r_1' are related to the corresponding r_0 and r_0' values at the entrance by the linear equations:

$$r_1 = a_{11} r_0 + a_{12} r_0'$$
$$r_1' = a_{21} r_0 + a_{22} r_0' \tag{7}$$

Using matrix notation we can rewrite this equation as

$$\mathbf{r}_1 = \begin{bmatrix} r_1 \\ r_1' \end{bmatrix}$$
$$\mathbf{r}_1 = \mathbf{A}\mathbf{r}_0 \tag{8}$$
$$\mathbf{r}_0 = \begin{bmatrix} r_0 \\ r_0' \end{bmatrix}$$

In this way we can trace a ray through any number of optical elements by simply multiplying the corresponding matrices, and can approximate the shape and size of the beam cross-section. A problem arose from the fact that the trajectory and the transfer matrix both depend on the focusing potential and on the particle energy. To handle these dependences relative quantities are used. The anode (for ion optics) or the cathode (for electron optics) is

considered to be on unit potential (i.e. the energy of the particles emerging from the cathode or anode is unity) and all other potential values are expressed in such units. Let us consider for instance a simple aperture lens, and its calculated potential function. If we reduce the focusing potential — say — to 50% of its previous value, we have to multiply the potential distribution function by the constant value of $c = 0.5$. If the particle energy is changed by $\Delta\rho$ (electron volts), that change is equivalent to changing the electrostatic focusing potential by $\Delta\rho$ (volts), so we can take into account the difference in the energy of the incoming particles by simply multiplying the potential function by a suitable c value. The *GUNSMITH* can compute all the first order optical properties as a function of c, and can calculate the derivates of these quantities which express the chromatic aberration. Because the CAD system is able to follow the trajectory of the charged particles it is also capable of calculating the particle density distribution in any cross-section of the particle beam. For this calculation a number of particles is traced through the system from an arbitrary cross section to another arbitrary cross section. The starting particle distribution and velocity distribution can be read from disc, or can be predefined (homogeneous or Gaussian particle distributions).

III. Description of the CAD system

The system modules

The CAD system is written in Turbo Pascal Version 5.0 and it consists of several co-working modules, linked together by the menu system. There are the following modules:

Data input module

This module performs the interactive data input for the other modules. With it the user can
— enter lens parameters, modify and delete lenses
— connect lenses to create a compound lens

Field computation module

This module calculates the charge density and the potential distributions.

Trajectory tracing module

This module traces the trajectories of sample particles and computes the first order optical properties and the chromatic aberration of the given lens system.

Optic composer module

This module enables the user to determine the lens matrix of a compound lens from the lens matrices of the constituents.

DBMS module

This module performs the management and maintenance of the lens data stored in the data base. The data base contains the electrode positions and voltages, the potential distributions, the lens matrices and their derivates. The user can use data already in the data base in his/her calculations either as it is, or combined with new data. The content of the data base can also be modified, new data can be added to, or old ones can be deleted from it.

Output module

Produces the output data or the results of the calculations in various modes. It can print them in tabular or graphic form onto the screen or printer.

Operation system module

This module makes possible to use the facilities of the DOS operating system, such as: examining directories, copying or deleting files, etc.

System usage

The first step in the design of a charged particle optic is the field computation. For this the CAD system requires the following data:
1. the gun shape, electrode positions in cylindrical coordinates,
2. the voltages of the electrodes in relative units, and
3. the sectioning of the electrodes.
The data input is interactive, the electrode positions can be monitored on-screen. New lens systems can be created by using predefined simple or compound lenses or by creating new lens elements. The accuracy of the calculations performed on a long beam transport system can be increased by dividing the system into two or more sections and calculating the potential for each section, then fitting the resulting potentials together. Using the results of the field computation program the axial and radial potential distribution and the potential of any points are available and can be graphically displayed

on-screen. The second step in the design is the trajectory tracing. The data requirements are the following:

1. the z coordinates of the entrance and the exit planes of the optical system
2. the value of c, or the range of the allowed c values.

All the first order optical properties, their derivates and the chromatic aberration coefficients are a function of c and are presented in tabular form. The system can calculate the particle density distribution in the ion or electron beam too and these results are presented in graphical form.

The CAD system requires 640 kbytes memory and the computation times on an IBM AT without a 80287 math co-processor chip are the following:

$$\text{Field computation} \quad 20\text{---}60 \text{ minutes}$$
$$\text{Trajectory tracing} \quad 2\text{---}60 \text{ minutes}$$

The field computation time depends on the sectioning of the electrodes, while the trajectory tracing time depends on the range of c.

IV. Results

This CAD system has been used to simulate some double and triple cylinder and aperture lenses and the SIMS ion gun. The following tables and figures show our results and the comparisons with the literature.

SOME TRAJECTORIES THROUGH THE SIMS ION
GUN

Table 1

Properties of a double cylinder lens (See Fig. 1.) computed
with the GUNSMITH

c	V2/V1	F1	F2	CAPF1	CAPF2
0.5	2	11.061	15.646	13.220	13.087
0.8	5	1.769	3.959	2.789	2.482
0.9	10	0.805	2.549	1.628	1.189

Table 2

The results of Harting and Read [2] (Appendix 1 p. A 1.3)

c	V2/V1	F1	F2	CAPF1	CAPF2
0.5	2	11.05	15.63	13.21	13.07
0.8	5	1.77	3.95	2.78	2.48
0.9	10	0.80	2.54	1.62	1.19

Table 3

Properties of a double cylinder lens (See Fig 2.) computed with the GUNSMITH

c	V2/V1	F1	F2	CAPF1	CAPF2
0.5	2	13.007	18.393	15.398	15.533
0.8	5	2.007	4.486	3.022	2.955
0.9	10	0.892	2.819	1.666	1.453

Table 4

The results of Harting and Read [2] (Appendix 1. p. A 1.23): The mean deviation between our results and those of Harting and Read is 1.31 %

c	V2/V1	F1	F2	CAPF1	CAPF2
0.5	2	13.01	18.39	15.39	15.53
0.8	5	2.00	4.48	3.02	2.96
0.9	10	0.89	2.82	1.66	1.45
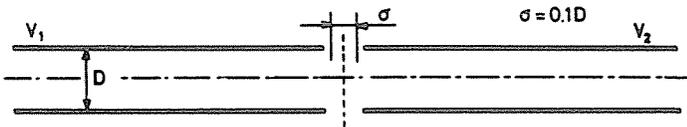
Fig. 1. Double cylinder lens, using equal diameter cylinders with thin walls. The fundamental unit of length is the diameter D, the length of the gap is $G = 0.1D$. The potentials of the cylinders are $V1$ and $V2$. $F1$, $F2$ are the focal lengths and CAPF1, CAPF2 are the mid-focal lengths
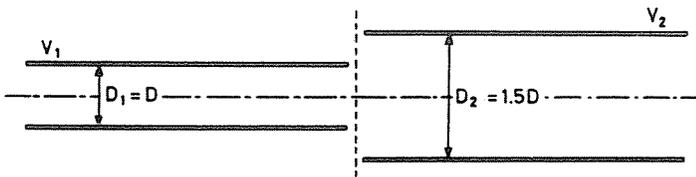
Fig. 2. Double cylinder lens using tubes of unequal diameters with thin walls

File name: IONF1.
Name of the optic: Ion source
The coordinate system :   Axial potential distribution:
      $z_{min.}$ = -10.000   Minimum: $u_{min.}$ = 0.000
      z_{max} = 20.000   Maximum: $u_{max.}$ = 0.999
      $r_{max.}$ = 15.000
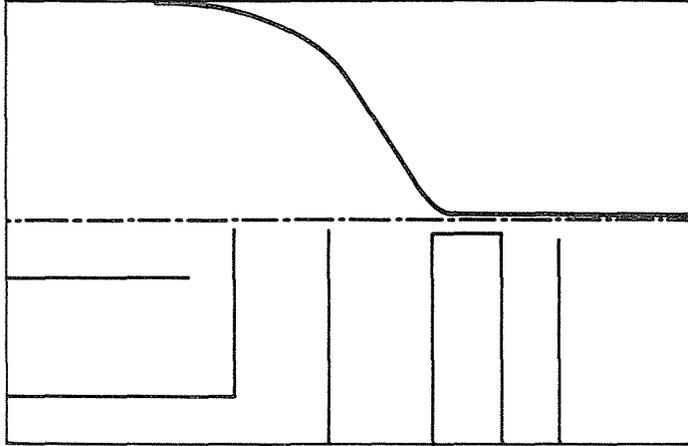
Fig. 3. The axial potential distribution of the SIMS ion gun, section I

File name: SIMS1.MAT
Name of the optic: sims1
The source:
File name of the source: ION.SRC
The distribution is homogeneous: The coordinate system:
Number of the particles = 100 $z_{min.}$ = 0.00
             $r_{max.}$ = 0.500 z_{max} = 180.00
    Angle range % (•) = 10.000 $r_{max.}$ = 4.00
    Angle range % (-) = 10.000
    Range of c % (•) = 5.000
    Range of c % (-) = 10.000

c = 0.70
α = 51.00%
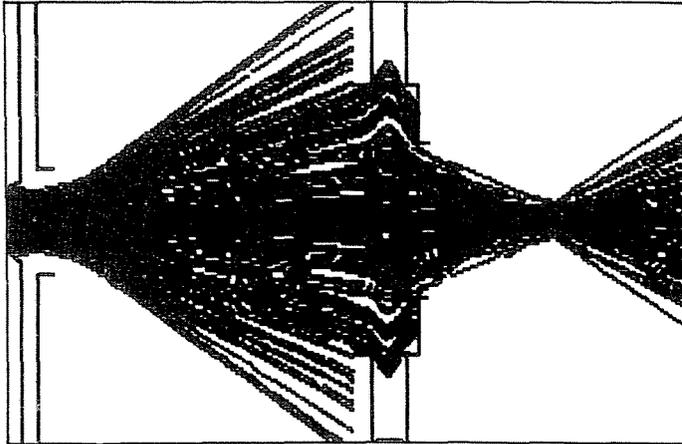
Fig. 4

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A. HAVAS
A. SÓLYOM
G. HÁRS
L. BORI
} H-1521, Budapest