technical memorandum Daresbury Laboratory

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A FORTRAN PROGRAM FOR THE CALCULATION OF ELECTRON TRAJECTORIES IN ELECTROSTATIC CYLINDER LENSES

by

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1. INTRODUCTION

Electrostatic cylinder lenses have been extensively used in electron spectroscopy for imaging electrons of variable energy from a fixed object point to a fixed image point. The basic units of the electron optical systems have been two and three element cylinder lenses as their relevant properties have been tabulated[1]. For designing more than three element systems and for investigatng more fully the action of simple lenses a comprehensive computer simulation of the electron trajectories has been developed. The program is an extension of the method developed by Fink and Kisker[2,3].

2. SCOPE OF THE PROGRAM

The program is able to perform four different ray-tracing tasks.

(1) Plot the trajectory of an electron through a tube lens system from a definsd starting radius and slope in the object plane.

(2) The object is assumed to be a gaussian source of electrons with a definsd full width at half maximum and angular divergence. Electrons from the object plane are mapped through to the image plane and a graph is produced of electron density against radial position. A large number of radial positions are chosen in the object plane so that for good focusing a good representation of a gaussian is produced in the image plane. This option also calculates the percentage transmission through a defined aperture size in the image plane.

(3) The object again is described by a gaussian as in (2) but only 21 points are used in the object plane. An image plane electron density plot is produced which allows each of the 21 focal spots to be examined. In this manner, off axis imaging quality can be measured.

(4) Three points only are used in the object plane, one on the axis and one each on the full width at half maximum points. The full width at half maximum and the angular divergence are defined with 22 electrons from the axis and 11 from each of the FWHM points. These electrons are distributed equally in angle within the defined divergence and their trajectories are drawn from the object to the image plane.

The following restrictions apply to the program.

(a) Up to 36 elements may be used.
(b) Any individual tube must be less than 100 radii long.
(c) The total length of the system must be less than 270 radii.
(d) All cylinders must be of the same radius.

The program is written in Fortran 77 with Ghost graphics and runs on a DEC VAX 750.

3. THEORY OF ELECTRON TRAJECTORY CALCULATION

The calculation of electron trajectories in an electrostatic field is divided into two separate steps. The potential distribution is first found and then the equation of motion of the electron within the field is solved. In a cylindrical electrostatic system the scalar potential field may be expressed by Laplaces equation in the form,

$$\nabla^2 v = \frac{\partial^2 v}{\partial r^2} + \frac{1}{r}\frac{\partial v}{\partial r} + \frac{\partial^2 v}{\partial z^2} = 0 \qquad (1)$$

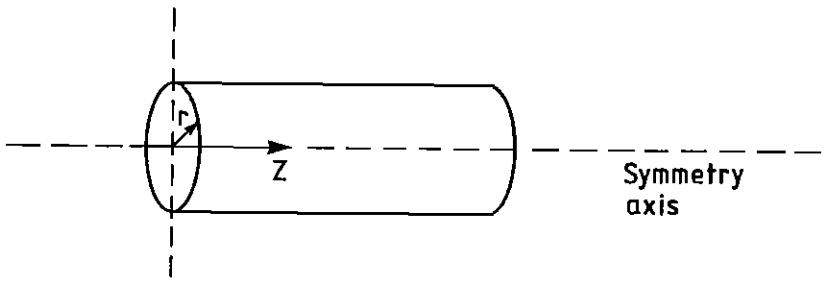


Fig.1

where V = V(r,z) is the scalar electric potential.

r is the radial coordinate

z is the axial coordinate taken from a reference plane.

Following the paraxial approximation method of Bertram[4] it is sufficient to calculate only the axial potential distribution,

$$V(r,z) = V(z) \tag{2}$$

The solution of equation (1) can be expressed as a Fourier integral

$$V(r,z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} a(k)\, I_0(kr)\, e^{ikz}\, dk \tag{3}$$

where $I_0(kr) = J(ikr)$, a Bessel Function of zero order and imaginary argument.

The functions a(k) are chosen to fit the boundary conditions and are calculated by taking a Fourier transform in terms of the boundary potential V(R,z). By expressing the system radius as R=1, the functions a(k) may be found and if the potential gradient at the boundary r=R is assumed to be constant an expression may be found for the potential in two adjacent cylinders[5].

$$V(r,z) = VA + \frac{VB - VA}{g} \left[U_1(r, z + g/2) - U_1(r, z - g/2)\right] \tag{4}$$

where g = width of the gap in terms of R.

VA = first lens potential.

VB = second lens potential.

The terms $U_1(r,z)$ are independent of the potential and may be expressed as,

$$z + \sum_P \frac{J_0(Pr)}{\mu^2 J_1(P)}\, e^{-Pz}, \qquad \text{For } z > 0 \tag{5}$$

$$\sum_P \frac{J_0(Pr)}{\mu^2 J_1(P)}\, e^{Pz}, \qquad \text{For } z < 0 \tag{6}$$

where J_0 and J_1 are Bessel functions of zero and first order respectively: p are the roots of $J_0(p) = 0$. As stated earlier, if a paraxial approximation is used, only the potential along the axis is required and hence we only need $U_1(0,z)$. These unified potentials have been tabulated[4] and are in integral steps of R/20 up to 3/2 R; for z greater than 3/2R the terms $U_1(z)$ are extrapolated as $0.332\, e^{-2.4z}$.

The potentials in more than two element systems are calculated by superimposing adjacent lens potentials as shown in fig.2.

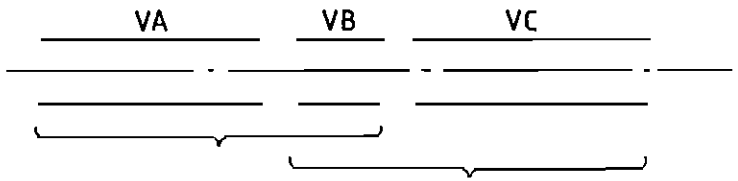


Fig.2

In this case the potential B is calculated by superimposing the two potentials for AB and BC.

The equation of motion of a single electron in a cylindrically symmetric electrostatic field is given by[5]

$$\frac{d^2r}{dz^2} + \frac{1}{2V}\frac{dV}{dz}\frac{dr}{dz} + \frac{1}{4V}\frac{d^2V}{dz^2}(r) = 0 \tag{7}$$

where V is the axial potential V(0,z).

Substitution in eq(7) for r in terms of the reduced radius R_d gives

$$\frac{d^2 R_d}{dz^2} + \frac{3}{16}\left(\frac{1}{V}\frac{dV}{dz}\right)^2 R_d = 0 \tag{8}$$

where the reduced R_d is given by

$$R_d = r\, V^{1/4} \tag{9}$$

and in eqs.(7), (8) and (9) $V = V(z)$

Equation (8) can be iteratively solved using the Runge-Kutta method so that with knowledge of the radial starting position and the starting slope the reduced radius R_d can be found. The actual position of the electron r at any z can be found from eq.(9). The integration step used in the Runge-Kutta method has to be twice the step in the potential calculation. If I denotes the iteration step for the potential then the reduced radius can be expressed as,

$$R_d(I+2) = R_d(I)\left[1 - \frac{h^2}{6}\left(T(I) + 2T(I+1) - \frac{h^2}{4}\,T(I)\,T(I+1)\right)\right] + C_d(I)h\left(1 - \frac{h^2}{6}\,T(I+1)\right) \tag{10}$$

where

$$C_d(I+2) = -\,R_d(I)\,\frac{h}{6}\left(T(I) + 4T(I+1) - \frac{h^2}{2}\,T(I)\,T(I+1)\right) + C_d(I)\left(1 - \frac{h^2}{3}\,T(I+1)\right) - \frac{h}{6}\,T(I+2)\,R_d(I+2) \tag{11}$$

$$R_d = \frac{r}{V^{1/4}} \qquad C_d = \frac{c}{V^{1/4}}$$

where r is the real radius, c is the real slope, R_d is the reduced radius and C_d is the raduced slope, and

$$T(I) = \frac{3}{16}\left(\frac{1}{V(I)}\,\frac{dV(I)}{dz}\right)^2 \tag{12}$$

The method is recursive in that previously calculated values of the reduced radius and slope are used in the calculation of the new values at the next z position.

4. PROGRAM OPTIONS

As described in section 2, four options are available for different typss of raytracing. Option 1 traces the path of a single electron of definsd starting slope and position and is particularly useful when investigating the focusing properties of many element lenses where fast computation is essential. Option 4 is an extension of option 1 in that electrons are traced from three positions in the object plane, one point on the symmetry axis and one point each on the half width at half maximum points of a gaussian intensity distribution of defined width. The electrons coming from each of the three points are divided equally in a defined divergence angle with 11 electrons from the off axis points and 22 from the on axis point. This option is used when it is necessary to measure the filling factor of the lens system. In options 2 and 3 the paths of the electrons through the lens system is not displayed but the distribution of electrons in the image plane is instead plotted. In option 3 the object is again represented by a gaussian intensity distribution of defined width and angular divergence but 21 object points are used equally distributed between the ±99% integrated intensity positions. The number of electrons originating from each point represents a gaussian intensity distribution with 558 coming from the on-axis point. This option is particularly useful for examining off axis imaging quality. Option 2 again represents the object by a gaussian intensity distribution but in this case 552 object plane points are used. From each of the 552 points 9 electrons are emitted filling the defined divergence in equal anglss and the gaussian distribution is formed by a non-linear distribution of points in the object plane, i.e. the number of emitting points in a fixed interval in the object plane represents a gaussian. This type of distribution is necessary, as part of option 2 gives the percentage transmission of electrons through an aperture of defined size. If only a small number of equally spaced points are used the integration step width in the image plane can give rise to a false representation of the intensity distribution. This option is used where an accurate representation of the efficiency of a lens system is required and is particularly useful for studies of electron transmission where the electron energy does not correspond to the focused energy. This is of importance where an energy dispersive multidetector follows the lens system[7].

5. PROGRAM STRUCTURE

The following information is stored in the form of block data

(1) The first 31 elements of the reduced potential.

(2) The positions from which electrons originate in option 3 in terms of one standard deviation.

(3) The number of electrons originating from the points described in (2).

(4) The number of positions for each integral step in the object plane for option 2.

The initially required input data is;

(1) The number of lens elements.

(2) The radius of the tube lenses. (All must be the same).

(3) The lens voltages.

(4) The lens gaps in terms of R. (Must be greater than R/20).

(5) The lengths of the lens elements in terms of R (must be iess than 100 R).

The program will then search for the longest lens element so that if necessary extra reduced potential values can be created by the method described in section 3.

The number of data elements required is given by,

$$20 \times \{\text{length of the longest lens in terms of R}\} + 20 \times \{\text{length of the previous gap in terms of R}\}$$

The options are now given and selection is made. The inputs corresponding to the various options are now made.

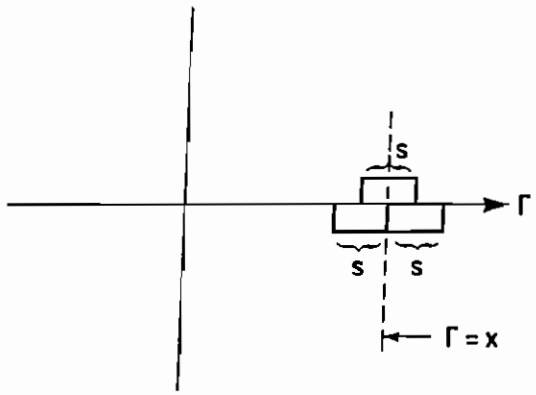
Option 1. The program requires the initial radius and slope of the electron trajectory.

Options 2, 3 and 4. The program requires the full width at half maximum of the object, the angular divergence from the object and the radius of the exit aperture.

If option 2 is selected, the number of electrons originating from each of the object steps is calculated so that the position of each object point can be found. The object points are equally distributed in space within each object step.

The program then calculates the potentials in pairs of lens elements. Using the superposition method given in section 3 the potentials are combined to yield the total system potential which ie stored in an array XX(I). The potentials in the lens gaps were calculated by assuming a constant potential gradient. A further array YY(I) was created for the potential gradients which were calculated simply by substraction of the I+1 and I-1 potential values divided by two step widths. The values T(I) in eq.(12) necessary for the Runge-Kutta integration were now calculated. The Runge-Kutta integration was then performed for each electron of different starting position and slope.

For options 1 and 4, the real radius at each integration step is plotted using GHOST graphics. For options 2 and 3 respectively, 4968 and 5515 electrons are traced through to the exit plane where their positions are stored. To produce an electron density plot, the integration step width is found from the maximum and minimum radial difference divided by 41. If the slope width is s and the position of the center of the integration is x then the integration is given by



$$\text{number at } r=x = \frac{1}{3}\left\{ \sum_{x-s}^{x} + \sum_{x-s/2}^{x+s/2} + \sum_{x}^{x+s} \right\}$$

Fig.3

where each summation represents the number of electrons in the defined interval. This is then found at all r in steps of s from the minimum to maximum r values. The electron density as a function of radial position is then plotted. The number of electrons occurring within the defined aperture radius are counted and printed on the electron density graph as a percentage of the total number of electrons from the object.

The program then gives the options

(1) Return to enter a new data set.
(2) Choose different output format.
(3) Change the voltages only.
(4) Exit the program.

6. TESTING OF THE PROGRAM

The program was tested against data tabulated for 2 and 3 element lenses by Harting and Read[1]. The first simple check was to compare the graphs of axial potentiale against those produced by the potential calculation of the program for the limited number of two and three element examples given. The results of the program were then checked by finding the principal planes, principal foci and image distance for a two element lens from the ray trajectories. The geometry of the image and object planes and the principal planes and foci are shown in fig.4.

The example given here is for a lens gap to diameter ratio (G/D) of 0.1 and an object distance to diameter ratio (P/D) of 2.0. In this example an acceleration ratio of 10:1 was used.

	Harting and Read[1]	Read et al[6]	Program
Q/D	7.8	-	7.83
F2/D	1.19	1.179	1.18
f2/D	2.54	2.528	2.52

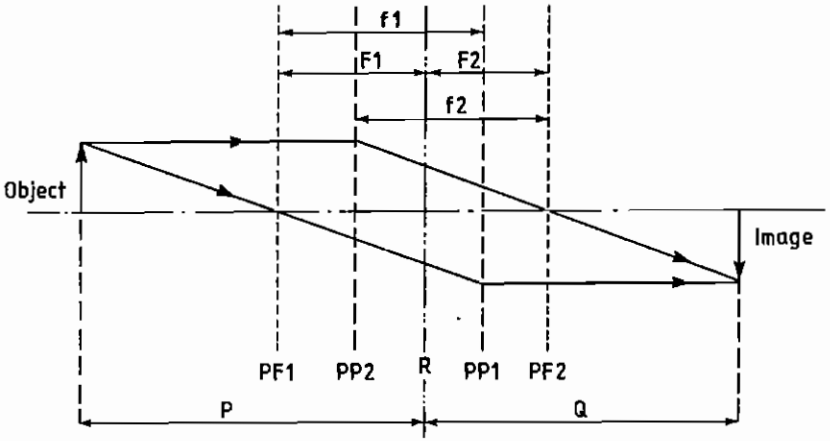
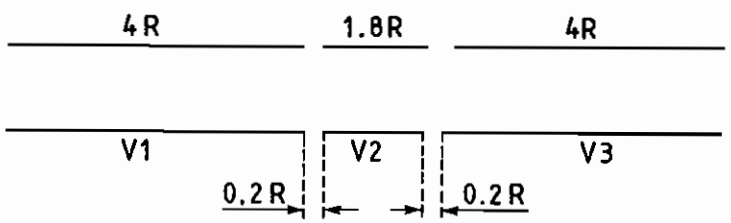


Fig. 4 Schematic representation of thick lens parameters
R; reference plane of lens (symmetry plane)
PP1, PP2; first and second principal planes
PF1, PF2; first and second principal foci
P,Q; conjugate object and image distances
D; lens diameter
G; lens gap

Numerous other focusing conditions were compared and always the agreement was better than 1%. A version of the program was written which allowed the focus voltage of a three element lens to be iterated until the best focus was obtained (see Appendix B). This was then used to produce lens tables of focusing voltage and magnification. An example of the comparison with the Harting and Read tables is given for the geometry shown in fig.5.



R; radius of tube

Fig. 5

V3/V1	V2/V1 (Program)	V2/V1 [1]	Mag (Program)	Mag [1]
3.0	0.212	0.2	0.65	0.7
	11.14	11.0	1.10	1.2
8.0	0.618	0.6	0.48	0.5
	13.21	13.4	1.05	1.1
16.0	1.572	1.5	0.43	0.45
	13.03	13.0	0.90	0.9

Note: lens voltages are referenced to the electron energy.

The agreement is within the increments of the tabulations in Harting and Read[1] and it should be noted that the program produces both the high and low voltage solutions. The high voltage solution would normally be used as the filling of the lens is less in this mode leading to less aberration. Further examples of the use of the program are given in Appendix C.

SUMMARY

The electron optics ray tracing program BEAM provides a powerful way to optimise the action of cylinder lenses. The program can be used interactively for the rapid design of simple lens systems or for more complex arrangements or iterative optimisation of lens voltages, the program is used in a batch mode. Several versions of the program exist for the optimisation of three and four element lens parameters. The programs may also be used for studying the transport of electrons of non-optimal energy as occurs in lens systems supplying electrons to energy dispersive analysers equipped with parallel readout[7].

Running the Program

The program is written in FORTRAN77 and runs under VMS version 4 on a DEC VAX.

The program is executed by typing,

'RUN BEAM'

The user is prompted for the number of elements.

'INPUT NUMBER OF LENS ELEMENTS (2-36)'

The radius of the tubes in millimeters is then required: NOTE: all the tubes must have the same radius.

'INPUT RADIUS OF THE TUBE LENS SYSTEM (mm)'

The program then requires the input of the individual lens voltages. Note: the voltages are always with respect to the electron energy.

'INPUT LENS VOLTAGES'

The lens gaps are then required. These have to be input as a fraction of the tube radius and must be a minimum of 1/20R and a multiple of this value. If a non integer value is chosen the nearest integer is used.

'INPUT LENS GAPS (IN TERMS OF R) (> 0.05 R)'

The lengths of the individual tube elements in terms of R is then required. The lengths should be an integer value of R/20; if a non integer value is defined, the nearest integer is used.

'INPUT LENGTHS OF LENSES IN TERMS OF R (< 100)'

The next prompt is for the required option. These options are as previously described.

'DO YOU REQUIRE
(1) A SINGLE ELECTRON TRAJECTORY
(2) BEAM PROFILE IN THE EXIT PLANE
(3) FOCUSING PROPERTIES IN THE EXIT PLANE
(4) SEVERAL ELECTRON TRAJECTORIES.'

Option 1: The program now requires the starting radius in mm and the slope in radians. The slope must be less than 0.17 radians.

'INPUT STARTING RADIUS (mm) and SLOPE (RADIANS)'

Options 2, 3 and 4: The program requires the FWHM spot size in mm and the divergence. Again, the divergence should be less than 0.17 radians.

'INPUT FULL WIDTH AT HALF MAXIMUM FOR THE SPOT IN THE ENTRANCE PLANE (mm)'

'INPUT FULL ANGULAR DIVERGENCE OF THE ENTRANT BEAM (RADIANS)'

For options 2, 3 and 4 the radius of the exit aperture in mm is required.

'INPUT THE RADIUS OF THE EXIT APERTURE, mm'

This is required so that the number of transmitted electrons can be calculated.

The final prompt is

'WOULD YOU LIKE TO,
(1) RETURN TO ENTER A NEW SET OF DATA
(2) CHOOSE DIFFERENT TREATMENT OF THE DATA
(3) CHANGE THE VOLTAGES ONLY
(4) EXIT THE PROGRAM.'

APPENDIX B

Different Versions of the Program

1. Focusing conditions for three and four element lenses.

Two programs exist for minimising the image plane spot size by varying the focusing voltages of the lens. The program ZX optimises the central element voltage for three element lenses and the program VARCOND optimises the two centre element voltages for a four element lens. The required inputs are,

(1) The lens gaps (in terms of R)
(2) The lens lengths (in terms of R)
(3) The first and last lens voltages.

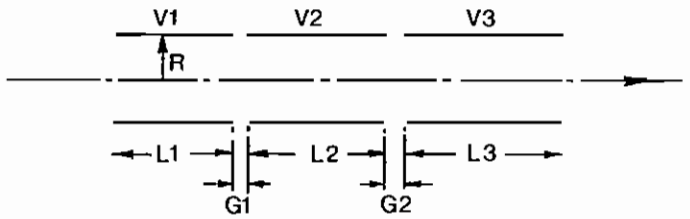
The central element voltages are iterated up to a maximum of 2000 V. The program may only be used in batch mode.

2. Transmission of a three element zoom lens for non-optimum electron energies.

The program PERCENT calculates the percentage transmission through a defined aperture in the image plane of electrons of energy within a defined range. The energy range and increment are defined by the user. The V1, V2 and V3 potentials are chosen so that usually the lens is in focus at the middle of the defined energy range. The program produces a plot of percentage transmission against electron kinetic energy. This program has been used to study the energy selection of three element zoom lenses in an attempt to define the useful operating ranges of following multichannel energy dispersive analysers. An example of its use is given in Appendix C.

APPENDIX C

The operation of the program is demonstrated in this section by application to a simple three element lens.



Example 1. The program is used to plot the trajectory of a eingle electron

V1 = 10 V V2 = 13.36 V V3 = 1 V
L1 = 4R L2 = 1.8 R L3 = 4 R
G1 = 0.2 R = G2

The initial radial position is 0.0 mm with an initial slope of 0.03 radians.

[PLOT 1]

Example 2. The program is used to plot several electron trajectories from three object plane points. The low voltage focusing solution is used.

V1 = 12 V V2 = 2.6 V V3 = 20 V
L1 = 6.9 R L2 = 1.8 R L3 = 4.9 R
G1 = 0.2 R = G2

The object is represented by three points with the outside points lying on the FWHM points of a Gaussian intensity distribution. The outside points have a separation of 0.5 mm and all three points have a divergence of 0.08 radians.

[PLOT 2]

Example 3. All parameters are the same as in example 2 except V2 which is 72.39 V and corresponds to the high voltage solution for focusing.

[PLOT 3]

Example 4. This demonstrates the use of option 2 in which a representation of the image plane intensity is given together with the number of electrons transmitted through a defined aperture in the exit plane. The lens parameters are the same as those in example 1 together with a spot size of 0.5 mm FWHM, an angular divergence of 0.08 radians and an exit aperture radius of 0.25 mm.

[PLOT 4]

Example 5. This demonstrates the use of option 3 which is used to study the focusing of a lens. Rays are traced from several object plane points representing a Gaussian intensity distribtuion to the image plane.

V1 = 12 V V2 = 86.14 V V3 = 40.0 V
L1 = 6.9 R L2 = 1.8 R L3 = 4.9 R
G1 = G2 = 0.2 R

[PLOT 5]

Example 6. The lens parameters are the same as for example 5. In example 5 V1 was 12 V which meant that the initial kinetic energy was 12 eV. In this example an 11.2 eV electron is traced through the same lens optimised for 12 eV. This is achieved by lowering all the potentials by 0.8 eV.

V1 = 11.2 V V2 = 85.34 V V3 = 39.2 V

Option 3 is used to demonstrate the defocusing effect.

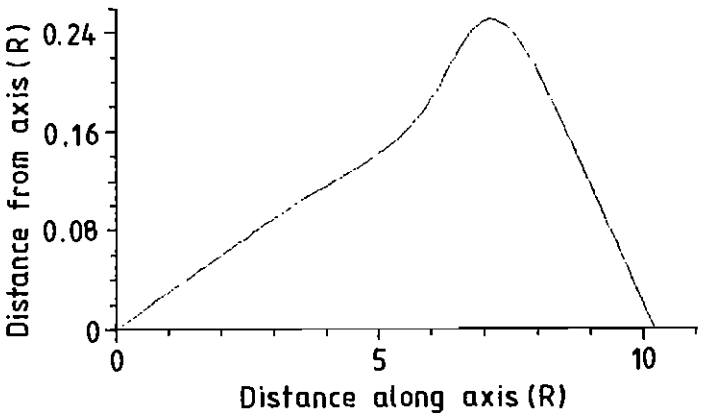
[PLOT 6]

Example 7. This demonstrates the use of the routine PERCENT. The lens has been focused for acceleration of 2.8 eV electrons to 20 eV. The number of electrons from a 1.0 mm object passing through a 0.5 mm hole in the image plane is plotted as a function of kinetic energy over a range from 1.0 eV to 4.6 eV. The defocusing of the lens can be clearly seen for non optimum energies.

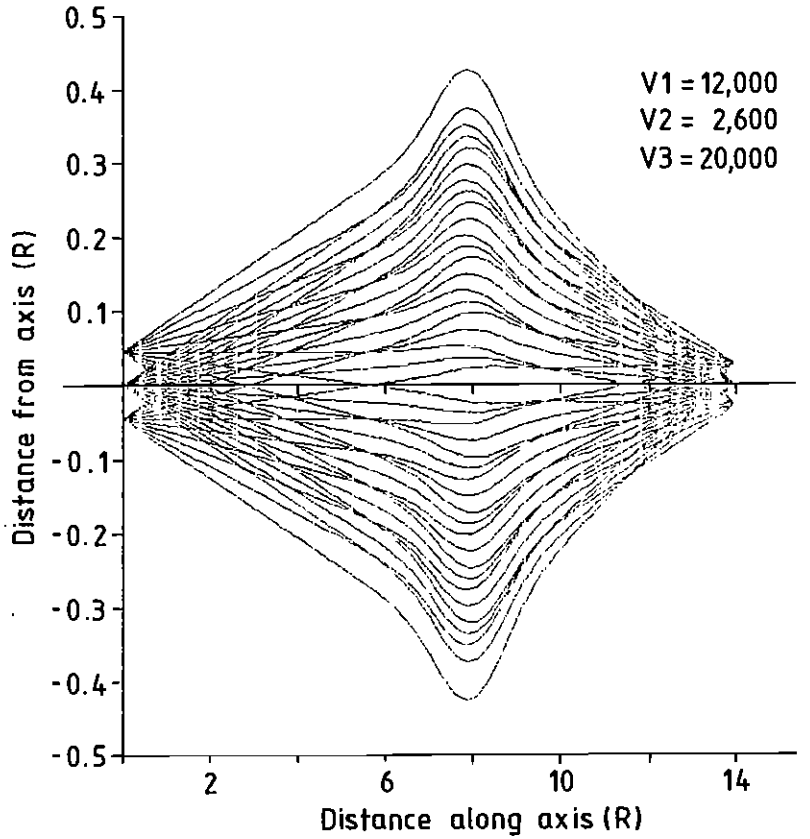
[PLOT 7]

REFERENCES

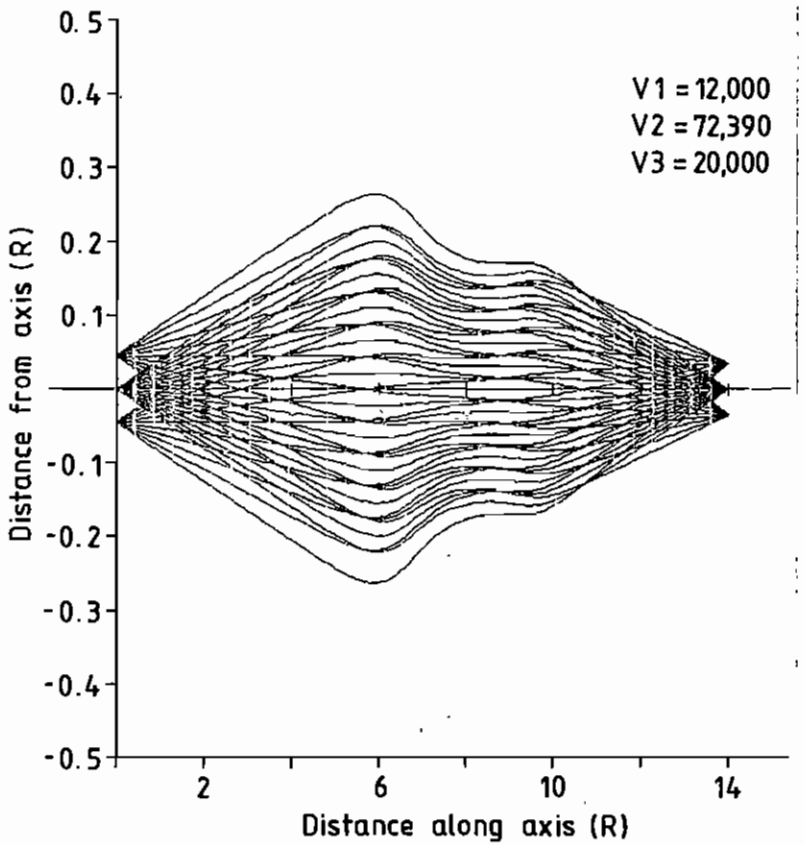
1. E. Harting and F.H. Read, 'Electrostatic Lenses' (Elsevier 1976).
2. J. Fink and E. Kieker, Rev. Sci. Instrum. 51, 7 (1980) 918.
3. E. Kisker, Rev. Sci. Instrum. 53, 1 (1982) 114.
4. S. Bertram, J. Appl. Phys. 13 (1942) 496.
5. P. Grivet, 'Electron Optics' (Pergamon, Oxford 1965).
6. F.H. Read, A. Adams and J.R. Soto-Moutiel, J. Phys. E. 4 (1971) 625.
7. T.S. Padmore, M.A. Hoyland and H.A. Padmore, to be published.


Distance from axis (R)
0.24
0.16
0.08
0
0
5
10
Distance along axis (R)

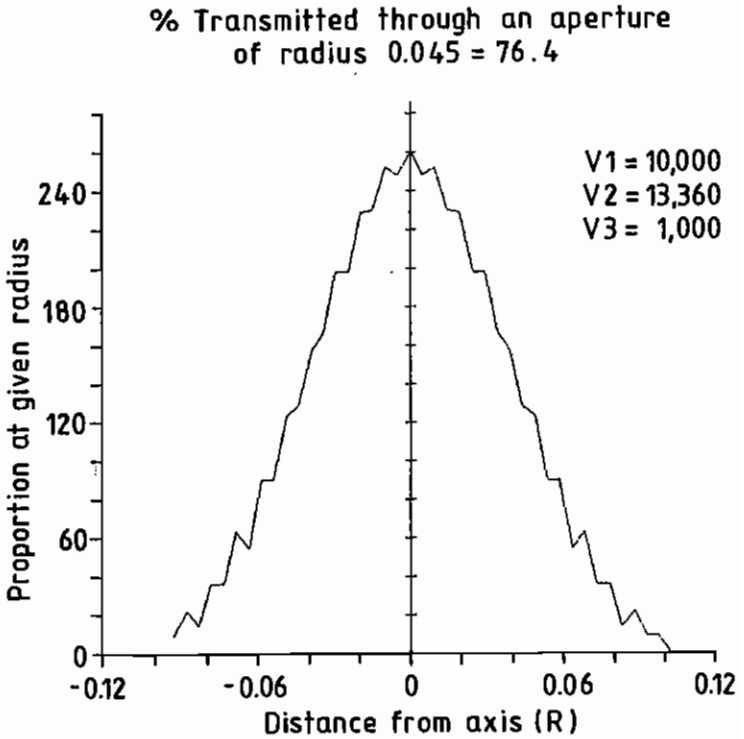
Plot 1


V1 = 12,000
V2 = 2,600
V3 = 20,000
Distance from axis (R)
0.5
0.4
0.3
0.2
0.1
-0.1
-0.2
-0.3
-0.4
-0.5
2
6
10
14
Distance along axis (R)

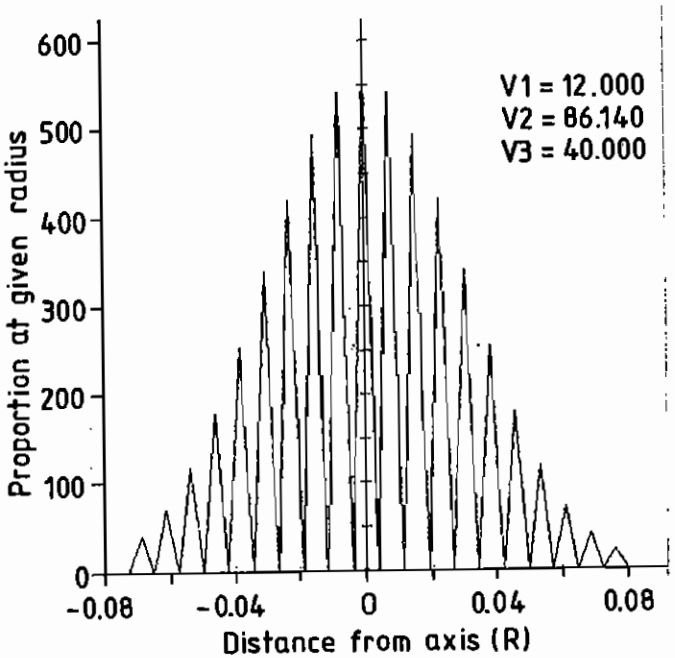
Plot 2


V1 = 12,000
V2 = 72,390
V3 = 20,000
Distance from axis (R)
0.5
0.4
0.3
0.2
0.1
-0.1
-0.2
-0.3
-0.4
-0.5
2
6
10
14
Distance along axis (R)

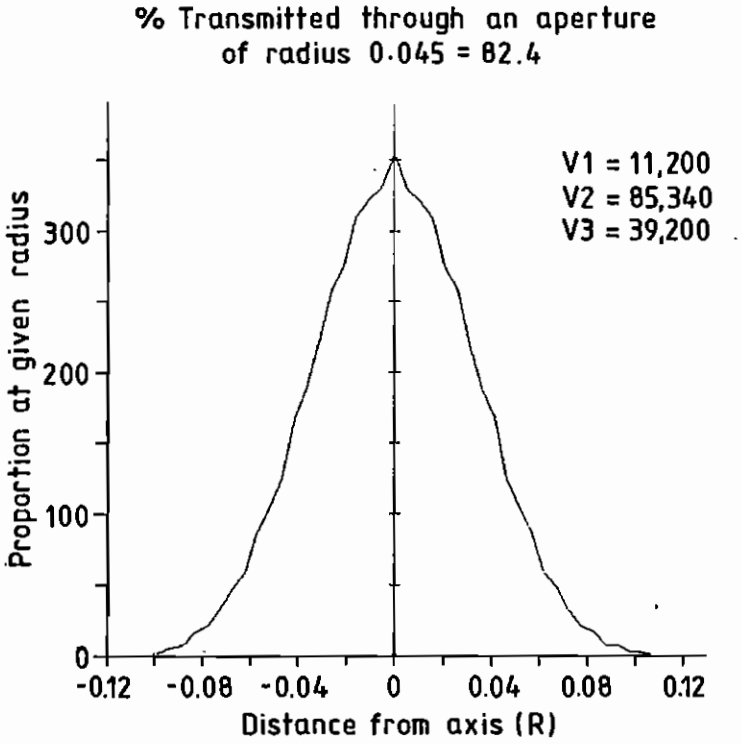
Plot 3


% Transmitted through an aperture
of radius 0.045 = 76.4
V1 = 10,000
V2 = 13,360
V3 = 1,000
Proportion at given radius
240
180
120
60
0
-0.12
-0.06
0
0.06
0.12
Distance from axis (R)

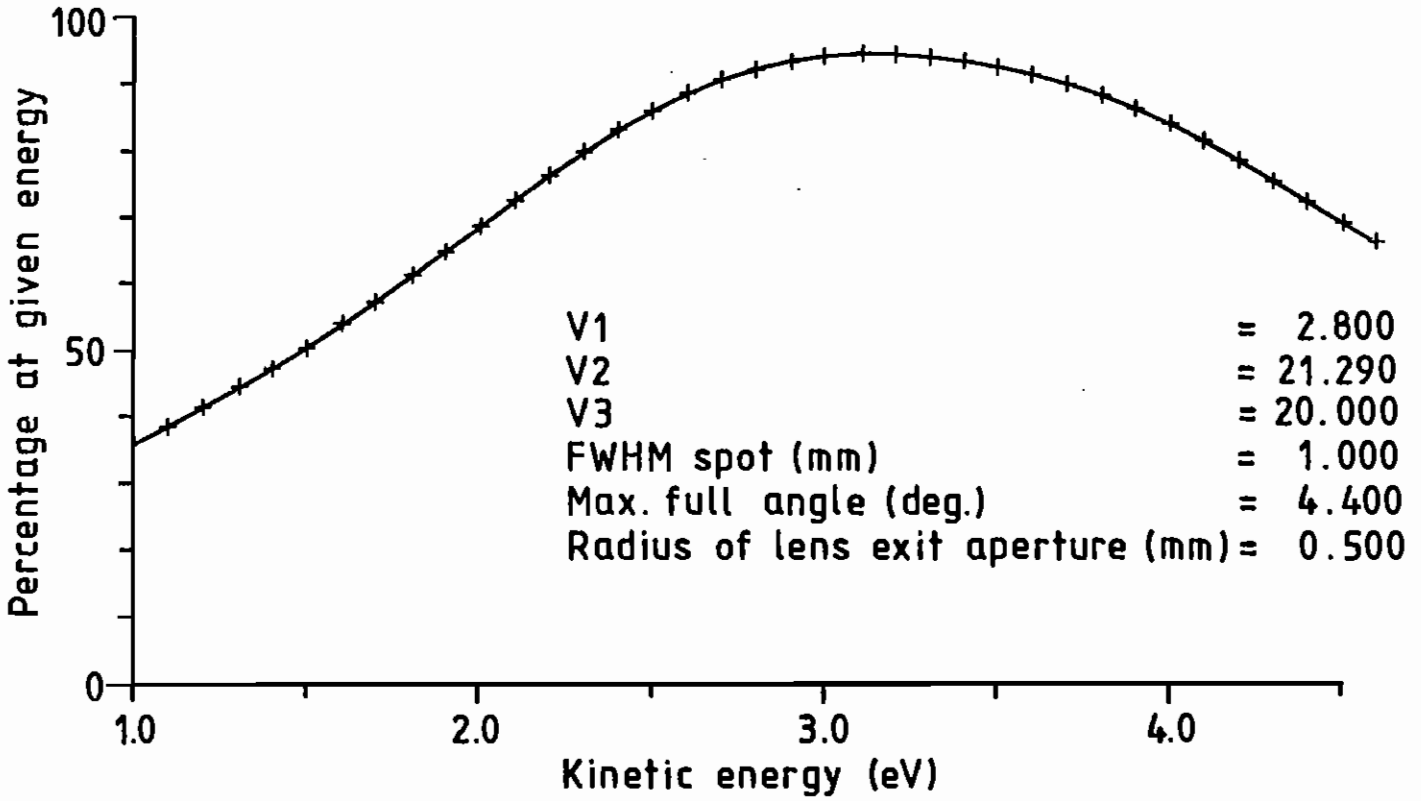
Plot 4


V1 = 12.000
V2 = 86.140
V3 = 40.000
Proportion at given radius
600
500
400
300
200
100
0
-0.08
-0.04
0
0.04
0.08
Distance from axis (R)

Plot 5


% Transmitted through an aperture
of radius 0.045 = 82.4
V1 = 11,200
V2 = 85,340
V3 = 39,200
Proportion at given radius
300
200
100
0
-0.12
-0.08
-0.04
0
0.04
0.08
0.12
Distance from axis (R)

Plot 6


100
50
0
Percentage at given energy
1.0
2.0
3.0
4.0
Kinetic energy (eV)
V1 = 2.800
V2 = 21.290
V3 = 20.000
FWHM spot (mm) = 1.000
Max. full angle (deg.) = 4.400
Radius of lens exit aperture (mm) = 0.500

Plot 7