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Design of a 90 degree spherical deflection analyzer

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Abstract

Ray tracing calculations have been performed for a 90 degree spherical deflection analyzer taking into account realistic fringe fields. The results are compared with previous results which used approximations to account for the fringe fields' effects. A new mode of operation, which leads to higher resolution of the analyzer, was found and is discussed in detail.

Keywords: Equipment; Fringe field; Instrument; Novel; SDA-90

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1. Introduction

In 1919 Aston [1] pointed out that a section of a spherical condenser can be used as a focusing energy analyzer for charged particles. Then in 1938, Purcell [2] calculated the trajectories and showed that there is a focusing action in a plane through the axis. Ashby treated the relativistic case [3] and this treatment was extended by Kessler and Weichert in 1964 [4]. Purcell, in addition to Kessler and Weichert, constructed 90 degree sector spherical deflection analyzers (SDA-90s) and tested some of their theoretical results [2,4]. This type of analyzer has been used successfully in many applications to record electron energy spectra [5,6]. In the theory, non-relativistic electrons from a point source on the axis are brought back to a focus on the axis after passing through the concentric spheres, and relativistic electrons focus beyond the axis on a focal ring [3,4]. This particular property together with the high luminosity [7,8] make the SDA-90 very suitable for azimuthal angle analysis and as a pre-analyzer in a β-spectrometer. Here we report the results of extensive ray tracing calculations of this analyzer in several different configurations, avoiding many approximations previously used in analytical treatments.

Kessler and Weichert [4] have calculated the important parameters such as focal point position, dispersion, and resolution. They assumed a Coulomb field inside the spherical condenser and zero field outside. The effect of crossing the artificial boundary between the Coulomb field and the field free region is approximated by Snell's law of refraction, ignoring all fringe fields. We have found that the real fringe fields provide an additional mode of operation with better resolution than the idealized case. The focal point for the new mode is further beyond the axis than predicted by Kessler and Weichert [4].

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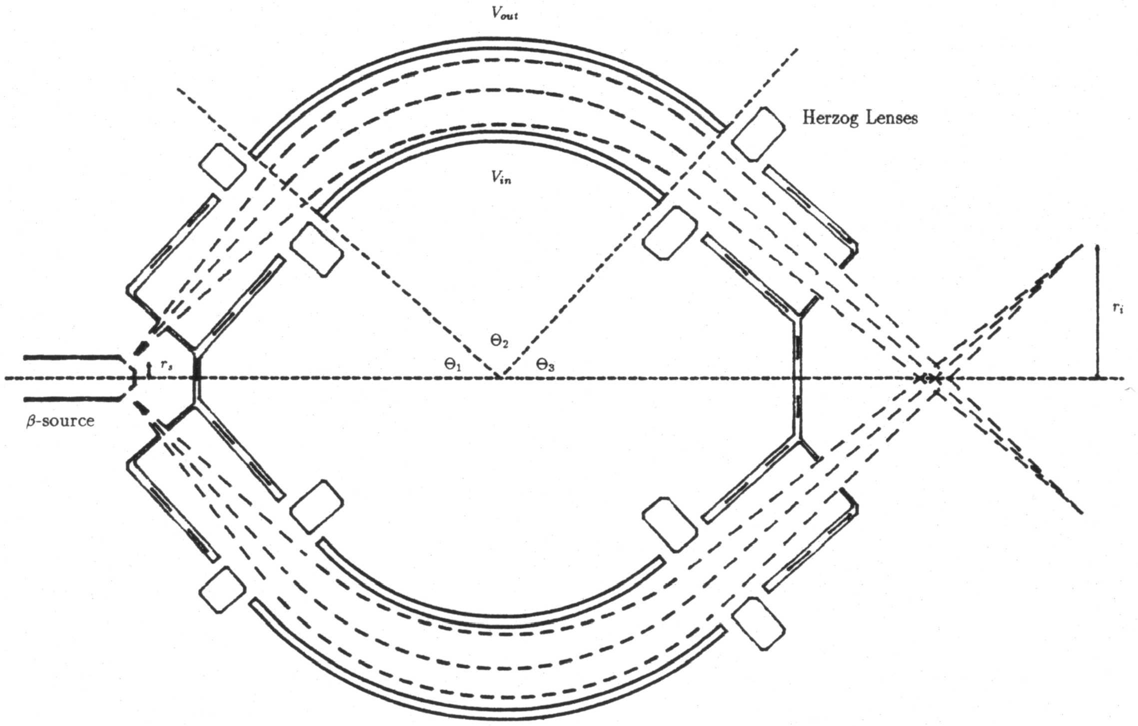

Fig. 1. Schematic diagram of the spherical deflection analyzer (SDA).

Although the primary objective of this analysis was to optimize the design for a specific application, a range of parameters was studied and those results are the basis of this report.

2. Design of the analyzer

This study was undertaken to find the optimum design of the SDA-90 to be used in an apparatus for analyzing the endpoint of the β spectrum of tritium. Molecular tritium contained in a cell with an annular slit of width s will emit β electrons into the aperture of the spectrometer with an angular spread (acceptance angle) of α. The ring image formed by the SDA-90 beyond the axis acts as the source for a cylindrical mirror analyzer (CMA) with a resolution of better than 2×10^{-4}. In order to obtain the optimum resolution in the CMA, the SDA-90 must be designed so that the electrons enter the CMA at an angle of 42° [9]. The resolution of the SDA-90 itself is not critical, but conditions which result in a minimum beam width and angle at the SDA exit, i.e. the CMA entrance, will optimize the resolution of the SDA/CMA system. In the β experiment it is also very advantageous to ensure that the electrons are not decelerated before they pass through the spherical portion of the analyzer. Therefore, asymmetric biasing (explained below) is of particular interest.

The basic design of the SDA is shown in Fig. 1. The analyzer consists of two concentric spherical sectors of angle θ_2 rotationally symmetric with respect to the Z axis. The Coulomb field between the two spheres is produced by an applied voltage V_D. The angle θ_2 was chosen to be 90° and θ_1 was chosen so that the electrons, upon leaving the analyzer, travel with an angle of 42° with respect to the axis, the optimum entrance angle of the CMA. r_s and r_i are the off-axis positions of the source and focal point (image), respectively. The ratio of the inner to the outer radius was chosen to be 3/4 so that there would be just enough room inside for the range of angular spreads α to be studied. Herzog style lenses [10–12] were added to the entrance and exit of the

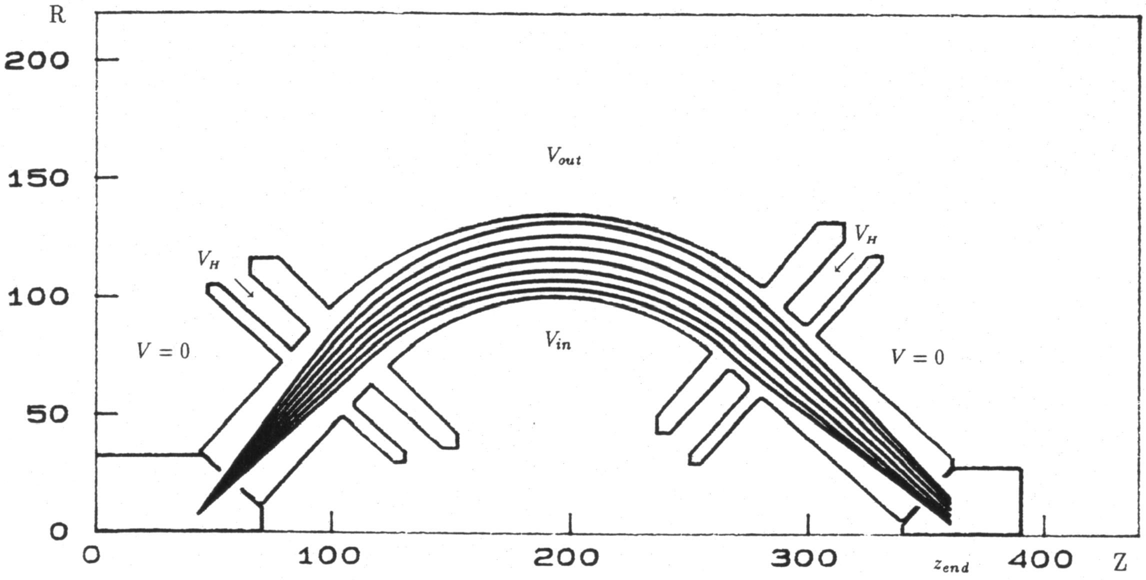

Fig. 2. Typical output of electron ray tracing program EGUN by Herrmannsfeldt [13]. The horizontal Z axis is the axis of cylindrical symmetry, and the vertical R axis is the radial coordinate. Axis units are in gridpoints with $R_0 = 117.75$. Traces are ended at the vertical cut at z_{end} which is in a field free region. Straight line trajectories are continued from this point to find the focal point.

analyzer to provide additional adjustability. As will be shown below, the purpose of these lenses will not necessarily be to correct the fringe fields, as is traditionally done.

In order to study the effects of the electrode voltages on the trajectories, it is convenient to use the quantities

$$V_{\text{offs}} = \frac{(V_{\text{in}} r_{\text{in}} + V_{\text{out}} r_{\text{out}})}{r_{\text{in}} + r_{\text{out}}} \tag{1}$$

and

$$V_{\text{D}} = V_{\text{in}} - V_{\text{out}} \tag{2}$$

where V_{in} and V_{out} are the voltages on the inner and outer spherical sectors with radii r_{in} and r_{out}, respectively. V_{offs} is the offset voltage of the analyzer, i.e. the amount by which the electrons of the central ray are accelerated before traversing the spherical portion of the analyzer, and V_{D} is the voltage to deflect the central ray along a circular trajectory. V_{offs} can be adjusted to select the optimum resolution; then V_{D} must be adjusted to obtain the proper trajectories. In this paper we present two particular arrangements: the case studied by Ashby [3] in which $V_{\text{offs}} = 0$ (we call this the "symmetric" case), and the case studied by Kessler and Weichert [4] in which $V_{\text{out}} = 0$ (the "asymmetric" case). In the analytical model, the voltages for the symmetric case are given by

$$V_{\text{D}} = \tfrac{1}{2}\beta^2 (V_{\text{e}} + m_0 c^2) \times \left(\frac{r_{\text{out}}}{r_{\text{in}}} - \frac{r_{\text{in}}}{r_{\text{out}}} \right) \tag{3}$$

$$V_{\text{in}} = \frac{V_{\text{D}} r_{\text{out}}}{r_{\text{out}} + r_{\text{in}}} \tag{4}$$

$$V_{\text{out}} = -\frac{V_{\text{D}} r_{\text{in}}}{r_{\text{out}} + r_{\text{in}}} \tag{5}$$

and for the asymmetric case by

$$V_{\text{D}} = V_{\text{in}} = -(V_{\text{e}} + m_0 c^2) + \frac{r_{\text{out}}}{r_{\text{in}}} \times \left\{ (V_{\text{e}} + m_0 c^2)^2 - \left[1 - \left(\frac{r_{\text{in}}}{r_{\text{out}}} \right)^2 \right] (m_0 c^2)^2 \right\}^{\frac{1}{2}} \tag{6}$$

$$V_{\text{offs}} = \frac{V_{\text{D}} r_{\text{in}}}{r_{\text{in}} + r_{\text{out}}} \tag{7}$$

In these equations V_{e} is the accelerating voltage, $\beta = \sqrt{1 - 1/\gamma^2}$, $\gamma = 1 + V_{\text{e}}/m_0 c^2$, and $m_0 c^2$ is the electron rest mass.

For our experiment the asymmetric case is desired for two reasons. Grounding the outer

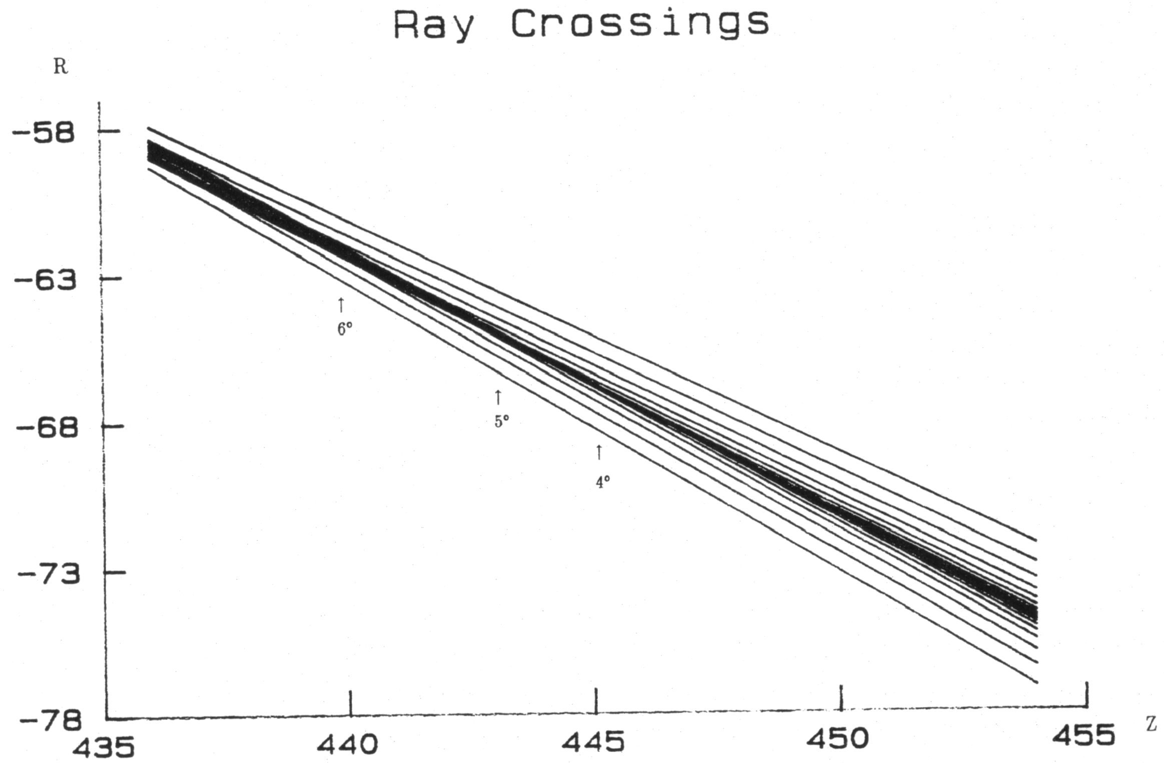

Fig. 3. The rays are shown in the focusing region beyond the axis (see Fig. 1). The minimum trace positions for 4°, 5° and 6° ray bundles with minimum trace widths of 0.121, 0.215 and 0.366, respectively, are also indicated. Axis units are in gridpoints.

sphere greatly simplifies the construction and mounting. More important, none of the electrons are decelerated as they enter the spherical part of the analyzer. Otherwise electrons formed inside the analyzer by β decay of the background tritium could interfere with the measurement of the end point of the tritium spectrum.

3. Procedure

A relativistic electron ray tracing program [13] was used to compute the electron trajectories in the SDA. A typical output is shown in Fig. 2. In this figure, Z is the axis of cylindrical symmetry and R is the radius. Calculations were performed on a DEC Microvax 3100-80 CISC running under the VMS 5.5-1 operating system. Typically 25 rays in steps of 0.5° were traced from a point source.

To find the image point and determine the optimum resolution, the coordinates of the rays are obtained at a vertical cut in the field free region at the location z_{end} shown in Fig. 2. Then a simple program is used to find the position of the minimum trace width measured parallel to the R axis for a range of different acceptance angles. For example, for an acceptance angle of $\alpha = 5°$ the program will find which 11 consecutive rays of the original 25, having a 0.5° spacing, will give the minimum trace width w_{min}, i.e. the smallest slit opening through which all rays will pass, and the location r_{min}, z_{min} where this occurs. The coordinates of this point (w_{min}, r_{min} and z_{min}), which actually represents an annular ring slit, are recorded. A typical output is shown in Fig. 3. The resolution $\Delta E/E$ (FWHM) was found by varying the energy of the electrons and observing the displacement of the image. ΔE then corresponds to the energy change required to move the center ray from one edge of the detector slit (w_{min}, r_{min}, z_{min}) to the other. This is justified because the rays are symmetrically distributed

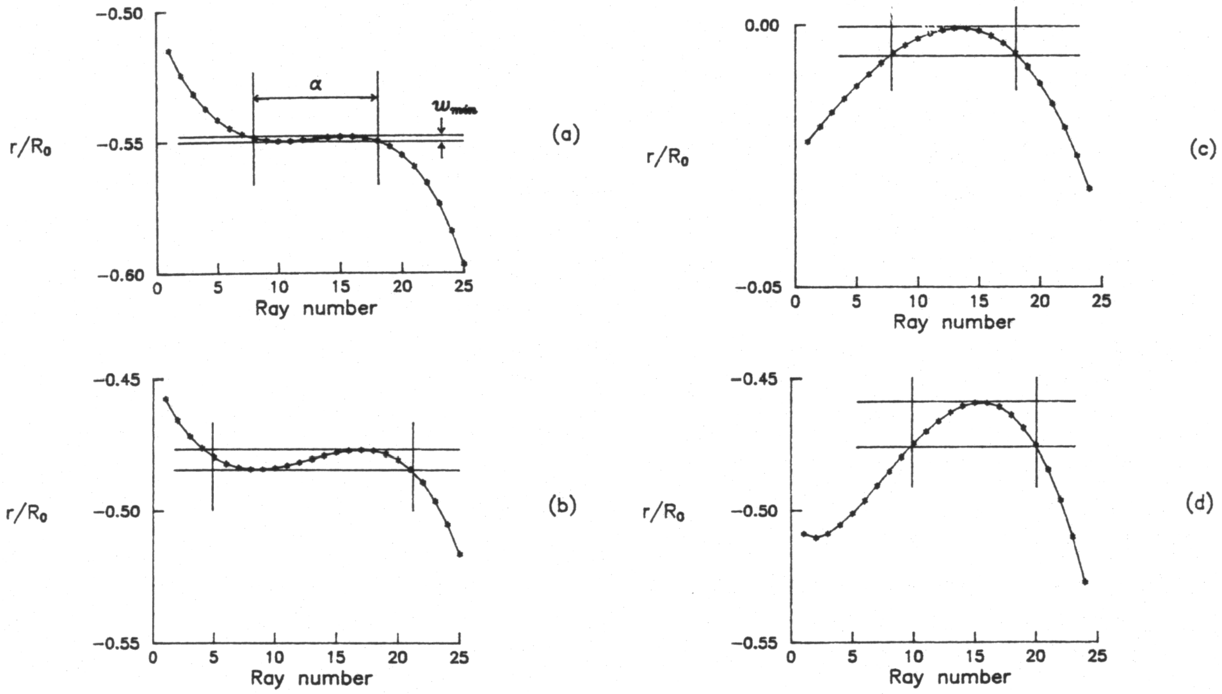

Fig. 4. Plots of r/R_0 versus ray number for ray bundles at the minimum trace position. These plots are used to determine the behavior of the trace width as a function of the acceptance angle α. (a) Asymmetric α^3 mode for $\alpha = 5°$. (b) Asymmetric α^3 mode for $\alpha = 8°$. (c) Analytical result of Kessler and Weichert [4] ($\alpha = 5°$). (d) Asymmetric α^2 mode ($\alpha = 5°$).

around the center ray and the intensity will be one half of the maximum at these two positions.

It can easily be shown that this method of calculating $\Delta E/E$ gives the value defined by Eqs. (1) and (2) of Kessler and Weichert [4] when the detector slit is set to the width and position of the minimum trace. This resolution is based on the source energy and not the pass energy.

To determine the effect of the finite size s of the source on the resolution, rays from points along the source slit (one from the middle and one from each edge) were traced, and the effect on the position of the image point observed.

Calculations were also carried out to test the results of Kessler and Weichert [4] in comparison to the results obtained using realistic fringe fields. A program was written based on the trajectory portion of the program SIMION [14], modified for relativistic electrons and for use of an analytical form for the potential rather than a potential array.

4. Results and discussion

Among all the parameters studied, the most important were the offset voltage V_{offs} and the mode of operation, which is determined by the minimum trace width chosen (there may be more than one). Other variables include the angles θ_1, θ_2, and θ_3, and the sizes of the gaps between the spherical portions and the grounded conical portions. All of these parameters can be varied to move the focal ring image to almost any desired location, but only the offset voltage and mode of operation affect the obtainable resolution.

The two modes of operation are characterized by the extent to which the resolution is affected by the acceptance angle α. In one mode, the resolution is approximately proportional to α^3, and in the other the resolution is approximately proportional to α^2. The most surprising result is that in the α^3 mode, a better resolution can be obtained than is predicted for the idealized cases studied by Ashby [3] and Kessler and Weichert [4]. This can be understood

Table 1
Voltages used to obtain the various analyzer modes for analyzing 18.6 keV electrons

Mode	V_{offs}	V_{D}	V_{H}	V_{in}	V_{out}
asym α^2	5873	13762	0	13762	0
asym α^3	5873	13762	0	13762	0
asym α^3 H	5936	13909	6000	13909	0
sym α^2	0	10673	0	6118	−4554
sym α^3	0	10673	0	6118	−4554
sym α^3 H	0	10555	−6000	6051	−4505

by looking at the caustic at the focal point. Figures 4(a) and (b) show the r coordinate of all of the rays versus ray number (i.e. entrance angle) at a fixed position z, corresponding to a minimum trace for two chosen α values, $\alpha = 5°$ and $8°$. These curves show that the minimum trace width depends on the cube of the source acceptance cone, α. Also shown in these figures are the exit slits w_{min} and the corresponding acceptance cones α defined by the entrance aperture and this slit. Since w_{min} is proportional to α^3, and since the resolution is proportional to w_{min}, the resolution is proportional to α^3. By comparison, Fig. 4(c) shows the same function ($\alpha = 5°$) as would be predicted for our analyzer by Ashby's equations [3].

If we switch the analyzer mode used for Fig. 4(a) to α^2 ($\alpha = 5°$) by choosing a different value of the Herzog lens voltage V_{H}, we get the result of Fig. 4(d). Note that the inflection point of the curve has shifted to the left and that the focal point has moved. The resolution obtained in this mode is worse than in the idealized case [3].

Table 1 shows some examples of the analyzer voltages used to obtain various modes of operation. The analyzer has been adjusted for detecting 18.6 keV electrons. An "H" in the first column indicates that the Herzog lenses were used to center the inflection point of the r versus ray number curve (see Fig. 4(a)).

Table 2 shows the positions of the focal points and the energy resolutions of the various modes shown in Table 1. It is common practice to parameterize the resolution as a function of the slit sizes and acceptance angle by the equation

$$\Delta E/E = As/R_0 + B\alpha^N \tag{8}$$

where s is the size of the source slit. The values of A, B, and N for the various modes are also shown in Table 2. Table 3 shows results obtained using the same methods for the analytical case studied by Kessler and Weichert [4], confirming their results.

As can be seen in the tables, the resolution is affected most by whether the α^2 or α^3 mode is used and by the value of V_{offs} (asymmetric or symmetric operation). It is very difficult to identify the individual parameters which are responsible for this behavior, since all parameters are highly correlated. Note, for example, that the use of the Herzog lens has only a small effect on the resolution, but a dramatic effect on the B parameter and in the focal point position during symmetric operation. The values of A, B, and N for the α^2 mode closely resemble the analytical results of Table 3, though the focal point positions do not match.

5. Conclusion

Our results show that a realistically modeled SDA-90 with fringe fields, when run in the α^3 mode, will have better resolution than is predicted

Table 2
Measured analyzer responses for the various modes obtained in Table 1; the value of s/R_0 is $0.45/117.75 = 3.8 \times 10^{-3}$

Mode	Focal point		$\Delta E/E \times 10^3$		A	B	N
	r/R_0	z/R_0	$\alpha = 2.5°$	$\alpha = 5°$			
asym α^2	−0.54	0.60	7.3	13.9	1.4	1.5	2.1
asym α^3	−0.62	0.69	6.0	8.9	1.4	2.4	2.7
asym α^3 H	−0.55	0.61	6.0	10.1	1.4	5.1	2.9
sym α^2	−0.78	0.87	6.5	13.5	1.0	1.0	1.9
sym α^3	−1.03	1.15	4.9	9.3	1.1	5.9	2.9
sym α^3 H	−0.52	0.58	4.9	9.1	1.1	2.6	2.6

Table 3
Analyzer responses for the ideal cases of Ashby [3] and Kessler and Weichert [4]

V_{offs}	V_D	r/R_0	z/R_0	$\Delta E/E \times 10^3$		A	B	N
				$\alpha = 2.5°$	$\alpha = 5°$			
6188	14501	0.00	0.00	6.99	13.06	1.3	1.1	2.0
0	10943	−0.17	0.19	5.81	11.24	1.0	1.0	2.0

by the analytical equations for the idealized analyzer having no fringe fields. When the real analyzer is run in the same mode as in the idealized case (α^2), the fringe fields degrade the resolution. However, the same fringe fields make the α^3 mode available so that higher resolution can be obtained.

The α^3 mode was not obtained in Kessler and Weichert's work [4] for two reasons. The most important is that it was not possible to place the detector at the minimum trace position in their apparatus. The other is that the inflection point of the ray number versus final position curve is not centred unless Herzog lenses are used or the source point is moved away from the ideal location.

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References

[1] F.W. Aston, Philos. Mag., 38 (1919) 710.
[2] E.M. Purcell, Phys. Rev., 54 (1938) 818.
[3] N. Ashby, Nucl. Instrum., 3 (1958) 90.
[4] J. Kessler and N. Weichert, Nucl. Instrum. Methods, 8 (1964) 245.
[5] D. Roy and J.D. Carette, Design of electron spectrometers for surface analysis, in H. Ibach (Ed.), Electron Spectroscopy for Surface Analysis, Springer-Verlag, Berlin, 1972.
[6] R.C.G. Leckey, J. Electron Spectrosc. Relat. Phenom., 43 (1987) 183.
[7] H. Hafner, J.A. Simpson and C.E. Kuyatt, Rev. Sci. Instrum., 39 (1968) 33.
[8] P.C. Kemeny, A.D. McLachlan, F.L. Battye, R.T. Poole, R.C.G. Leckey, J. Liesegang and J.G. Jenkin, Rev. Sci. Instrum., 44 (1973) 1197.
[9] H.Z. Sar-El, Rev. Sci. Instrum., 39 (1968) 533.
[10] R. Herzog, Z. Phys., 97 (1935) 596.
[11] R. Herzog, Phys. Z., 41 (1940) 18.
[12] H. Wollnik and H. Ewald, Nucl. Instrum. Methods, 36 (1965) 93.
[13] W.B. Herrmannsfeldt, Electron Trajectory Program, SLAC-Report-226, Stanford Linear Accelerator Center, Stanford University, Stanford, CA, 1979. Available from the National Technical Information Service, U.S. Department of Commerce, 5285 Port Royal Rd., Springfield, VA 22161.
[14] D.A. Dahl and J.E. Delmore, The SIMION PC/AT User's Manual Version 3.0, EG&G Idaho National Laboratory Informal Report EGG-CS-7233, 1987.