Novel toroidal electrostatic electron energy analyser

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Abstract: The characteristics of a novel, double toroidal, electrostatic electron energy analyser, with input and output optics, have been established. The energy and angular dispersed image on the surface of a microchannel plate detector enables parallel data processing and significant gains in efficiency. The characteristics of the toroids and lenses, including time dispersion, have been modelled using standard relaxation techniques and are compared with measured values. The calculations predict hemispherical radial magnification and second order focusing with 0.7% accuracy. The differences between point and distributed object sizes, such as may occur with solid and gas targets, are indicated. Measured elastic differential cross sections for 50 eV electrons scattered from argon and an Auger spectrum from argon are in good agreement with modelled data.

1. INTRODUCTION

The principles of toroidal, electrostatic deflection, particle energy analysers have been reviewed by Leckey [1]. Particles may be deflected with either radial or axial trajectories. Recently, radial deflection has been favoured, where particles scattered coplanar with the entrance slit are imaged for multi-parameter detection in an output plane. This feature enables electrons of the same energy, scattered through most angles from 0° up to 360° to be selected and focussed onto a circular line image at the output plane. Also the energy dispersed electrons will be imaged in a radial direction. With appropriate output optics and position sensitive detection of the electrons, such as with a microchannel plate, a map of the momentum dispersion of the selected electrons may be obtained. Such an instrument has considerable attraction because it permits essentially simultaneous detection of scattering events with consequential reduction in data gathering times. Such instruments have been developed by Engelhardt et al[2] and Leckey et al[3] for photoelectron spectroscopy using solid samples. The present instrument was developed for a gaseous target with some different requirements. This paper considers a model of important design features.

Our toroidal spectrometer was developed to study the electron impact ionisation of atoms and consequently there are at least two electrons emerging from the ionisation scattering process. Interest was confined to those events in which the energies of the two electrons were highly asymmetric which indicated two spectrometers were required. The small values of the triple differential ionisation cross sections implied that simultaneous rather than sequential data collection was necessary and the rapid decrease in those cross sections with increasing scattering angle meant that the higher energy analyser need only select scattered electrons from relatively small scattering angles. The interesting collision interaction mechanisms could be then explored by collecting the slower electrons over as much of 360° as

possible. From that basis a double toroid was designed with the inner toroid extending around 360° and the outer toroid from -30° to $+60^\circ$ with respect to the incident electron beam direction. The present paper concerns the modelling of the toroidal trajectories, output optics and the source and image characteristics and subsequent comparison with measured values.

2. THE MODEL

Figure 1 shows a planar cut through one half of the double toroidal analyser. Rotation of this section about the symmetry axis forms the toroidal geometry. The Inner Toroid (IT) has inner and outer radii of 45 and 55 mm respectively and a ratio of the cylindrical to hemispherical radii (a/b), c , as defined by Leckey[1], of 0.305. The source is defined by the intersection of an electron beam, 0.5 ± 0.1 mm diameter and the gas source which is modelled as a well defined profile or a uniform distributed background. The inner toroid has an input lens formed by cylindrical slits preceding the input slit S1 (0.25mm) which is not shown in the figure for clarity. The output optics L(N) are conical lenses which focus the image at the toroid output onto the surface of the microchannel plate (MCP) detector. The Outer Toroid (OT) has an inner and outer radii of 77.5 and 82.5 mm respectively and a , b and c parameters of 48mm, 80mm and 0.60 respectively. An input lens consisting of two cylindrical slits preceding slit S2' (0.5mm) is not shown for clarity. At the output of this analyser is a conical slit plate with discrete slits S2' (0.5mm) followed by channeltron detectors. Real slits S or radial slots are located at trajectory planes P(N). The trajectories of the fast electrons entering the outer toroid are perturbed by the inner toroidal field and the angle of incidence of the trajectories is not zero degrees, however these features have been successfully modelled.

The calculation of potentials and trajectories have been performed using standard relaxation techniques with a rectangular grid of dimensions up to 900×900 and cylindrical coordinates (Z, X, θ) with symmetry axis Z . The potentials and electric field along a given path were determined by using a third order Taylor expansion in Z and X with a uniform grid spanning the toroids and associated optics. The accuracy depends on the size of the grid and the curvature of surfaces. When the calculation was performed with boundary surfaces defined by grid points the accuracy was better than 0.05%. The radial dependence of the electric field was also determined for a hemisphere $a=0$, $b=50$ mm at angles of 0° , 70° and 180° ; the average deviation of the electric field from theory was 0.3%. The radial magnification was -0.993 , ie an error of 0.7% for an expected value of -1.0 . Trajectory calculations, out of the R, Z planes demonstrated second order focussing to an accuracy of better than 0.01 mm, a relative accuracy of 0.2%. The method and accuracy were also confirmed by repeating the similar calculations published by Hayes et al[4] in this laboratory for a hemispherical analyser for energy and time dispersion parameters. The calculations were made on a 33 MHz 486 computer using the Stanford 486 Fortran compiler, require 8Mbytes of RAM and includes screen graphics display. The results of these tests indicated a precision of better than 1% in calculating focussing parameters.

3. RESULTS

All of the modelled data refer to pass energies (E_0) through the inner toroid of 100 eV and outer toroid of 1000 eV. The performance of the analyser was evaluated for a range of focussing voltages (V) and an optimum focussing voltage ($V_0 = -72.42$ volts relative to ground, midway between the deflectors) was chosen which provided the best focussing and magnification characteristics for the MCP detector. Calculations were performed for values of r , defined as the ratio V/V_0 , between 0.7 and 1.2. If the c parameter and the ratio V/E_0 are held constant, the characteristics for various b and E_0 are found by applying an appropriate scaling factor; for example the energy dispersion curve for an analyser with $b = 150$ mm and $E_0 = 400$ eV would be $\partial R_{out} / \partial E_{in} = (150/50) \cdot (100/400) \cdot (\partial R_{out} / \partial E_{in})_0$. The transit time of the trajectories scales linearly with b and $1/\sqrt{E}$. The time dispersion is proportional to $\sqrt{E}$. The results of the calculations are presented in terms of the coordinates R , A , E , H and θ ; an explanation of these parameters and their relation to the μ, α, δ, v and β parameters of Wollnik[1] are given below. R is the displacement along the lines shown as P(N) in Fig. 1, for small deflections in-plane (in the ZX plane)

Fig. 1. Schematic of inner and outer toroids, trajectories and coordinates.

Fig. 2. Characteristics of Inner Toroid (IT) at P1(IT Input) $\circ$, P2(IT Output) $\blacksquare$, P3(Mask) $\blacktriangledown$, P4(MCP) $\blacklozenge$. See text for explanation of (a) to (e).

and out-of-plane (normal to ZX plane) this can be related to the μ parameter by dividing R by b for P1, P2, P5, and P6 and $\sqrt{2}b$ for P3 and P4. A is the in-plane angular displacement of the trajectory, and when defined in radians corresponds directly to the α parameter. E is the kinetic energy of the particles in eV and the δ parameter is equal to $(E - E_0)/E_0$. H is the horizontal or out-of-plane displacement and v is equal to H/b . The angular displacement θ is around the axis of symmetry. In all figures the solid lines are best polynomial fits to the modelled data and the dotted lines represent the limits on the parameters for this analyser due to the size of the source and input and output slits. All distribution widths quoted correspond to 2 standard deviations.

For small deviations of R the A and E response curves are sufficiently linear to describe the operating characteristics of the toroids and lens with a matrix formulation. Eqn. (1) is then constructed using linear fits to the data displayed in Figs. 2 to 6. The conversion to the optical matrices of Wollnik is readily accomplished by applying the following matrix multiplication. If C is the diagonal matrix eqn. (2b) whose elements equal the appropriate scaling factor between the associated parameters, say b_{in} for the R parameter at P2, then $M_{Wollnik} = CM_{Here}C^{-1}$. The in-plane matrix for the Inner Toroid IT is in reasonable agreement with calculations from Leckey[1], which were performed with and without terminating field corrections as described by Wollnik. The field corrected matrix gave the best overall agreement. The lens matrix L2 has been presented as a function of r, as shown in eqn. (3). IA represents the complete Inner Analyser and it can be seen in eqn. (4) that the parameters in L2(1)·IT closely approximate parameters in IA. Similar calculations have been performed for the outer toroid, in and out of the scattering plane. It should be noted that a combination of field termination problems and the non-circular orbit of the particles in the toroid leads to a small correction term of -0.044mm and 0.45 degrees at P2(IT output slit) and -0.144mm and -0.26 degrees at P4(MCP) for $r = 1$.

$$\begin{bmatrix} R_{out} \\ A_{out} \\ \Delta E_{out} \end{bmatrix} = \begin{bmatrix} (\partial R_{out} / \partial R_{in})_0 & (\partial R_{out} / \partial A_{in})_0 & (\partial R_{out} / \partial E_{in})_0 \\ (\partial A_{out} / \partial R_{in})_0 & (\partial A_{out} / \partial A_{in})_0 & (\partial A_{out} / \partial E_{in})_0 \\ (\partial E_{out} / \partial R_{in})_0 & (\partial E_{out} / \partial A_{in})_0 & (\partial E_{out} / \partial E_{in})_0 \end{bmatrix} \cdot \begin{bmatrix} R_{in} \\ A_{in} \\ \Delta E_{in} \end{bmatrix} \quad (1)$$

$$IT_{Here} = \begin{bmatrix} -0.997 & 0.027 & 0.756 \\ -0.621 & -0.985 & 0.309 \\ 0 & 0 & 1 \end{bmatrix}, \quad IT_{Leckey} = \begin{bmatrix} -0.90 & 0.062 & 0.72 \\ -0.66 & -1.06 & 0.25 \\ 0 & 0 & 1 \end{bmatrix} \quad (2a)$$

$$C = \begin{bmatrix} 50 & 0 & 0 \\ 0 & 57.3 & 0 \\ 0 & 0 & 100 \end{bmatrix} \quad (2b)$$

$$L2(r) = \begin{bmatrix} 8.84 - 11.54r & 4.68 - 4.75r & -0.009 + 0.015r \\ 8.90 - 13.64r & 5.04 - 5.73r & -0.009 + 0.016r \\ 0 & 0 & 1 \end{bmatrix} \quad (3)$$

$$IA = \begin{bmatrix} 2.663 & 0.007 & -2.081 \\ 5.124 & 0.568 & -3.854 \\ 0 & 0 & 1 \end{bmatrix}, \quad L2(1) \cdot IT = \begin{bmatrix} 2.74 & 0.000 & -2.06 \\ 5.155 & 0.555 & -3.79 \\ 0 & 0 & 1 \end{bmatrix} \quad (4)$$

If Gaussian responses are assumed the various contributions to the radial image can be added in quadrature as shown in eqn. (5) and eqn. (6). This gives a good estimate of the radial image size in each

Fig. 3. In - plane response curves for the conical lens for various ratios of the actual voltage to the optimum voltage on L2 ($V_0 = -72.42$). 0.7 $\circ$, 0.8 $\bullet$, 0.9 ∇ , 1.0 $\blacktriangledown$, 1.1 $\square$, 1.2 $\blacksquare$. See text for explanation of (a) to (f).

Fig. 4. Characteristics of Outer Toroid (OT) at P5(OT Output) with $\blacksquare$ and without $\circ$ a 100eV pass energy inner toroid deflection field. See text for explanation of (a) to (e).

analyser (ΔR_{IT} and ΔR_{OT}) and hence the ultimate resolving power given in eqn. (7). Only the significant contributions have been included for each analyser and this leads to different expressions for ΔR_{IT} and ΔR_{OT} .

$$\Delta R_{IT} = \sqrt{(M_R \cdot \Delta R_{in})^2 + (D_i \cdot \Delta E_{in})^2 + (C_{R,A} \cdot (\Delta A_{in} / 2)^2)^2 + (C_{R,H} \cdot (\Delta H_{in} / 2)^2)^2 + R_{grid}^2 + R_{det}^2} \quad (5)$$

$$\Delta R_{OT} = \sqrt{(M_R \cdot \Delta R_{in})^2 + (D_i \cdot \Delta E_{in})^2 + (C_R \cdot \Delta A_{in} + 2 \cdot C_{R,A} \cdot A_{in} \cdot \Delta A_{in})^2 + R_{det}^2} \quad (6)$$

$$\text{Resolving Power} = \frac{E_0}{\Delta E} = \frac{|D_i| \cdot E_0}{\Delta R_{IT/OT}} \quad \text{where } \Delta E_{in} = 0. \quad (7)$$

Fig. 2 shows the characteristics of the inner toroid at positions P1 to P4 and indicates the values of parameters in the above equation. In Fig. 2a, the radial magnification ($M_R = \partial R_{out} / \partial R_{in}$) at the toroid output plane (P1) is -1.00 and at the MCP image plane (P4) is 2.66 . In Fig. 2c, the energy dispersion ($D_i = \partial R / \partial E$) at P1 is 0.756 and at P4 is -2.08 . In Fig. 2d, the axial magnification M_H is given by $(\partial \theta_{out} / \partial H_{in}) \cdot (b \pm R_{out}) \approx -0.26$ at P1 and $(\partial \theta_{out} / \partial H_{in}) \cdot (\text{Image radius}) \approx -1.29$ at P4. In Fig. 2b it can be seen that a good focus exists at P; However, aberration effects shown in Fig. 2b and Fig. 2d arise from second order correlations between R with H and A; they become significant for extended sources and the contribution to the final image size is $R_{R,A} = C_{R,A} \cdot (\Delta A / 2)^2$ and $R_{R,A} = C_{R,A} \cdot (\Delta A / 2)^2$ where $C_{R,A} = 0.5 \cdot \partial^2 R / \partial A^2$, $C_{R,H} = 0.5 \cdot \partial^2 R / \partial H^2$ and the angular and source widths are ΔA and ΔH respectively.

For the inner analyser the source is significantly greater than the slit size so the effective width of the input slit is $\Delta R_{in} = 0.73 \cdot S1'$ and assuming an electron beam width, w of 0.5mm , the azimuthal spread is given by $A_{in} = 1.04 \cdot (w / a) \cdot (180 / \pi)$. Also, R_{grid} is the effective resolution of the histogramming grid and R_{det} is the resolution of the detection electronics. Ignoring second order effects and experimental resolutions we can see that the magnitude of the ratio of energy resolving powers at P4 and P2 is $|D_{i,P4} / (M_{R,P4} \cdot D_{i,P2})|$ and has a value of 1.03 . This shows that little energy dispersion occurs in the conical lens and the energy resolution is determined by the toroidal spectrometer, as expected.

The calculations performed for the complete analyser have been shown to be generally in good agreement with experimental results. For instance, experimental estimates of the energy dispersion D_i obtained by fits to argon Auger and helium autoionisation peaks agree with first order estimates and the full simulation to better than 5%. Estimates predicting the image size are less accurate due to the number of parameters which play an important role in determining the resolution, in particular the estimates of $R_{detector}$ which varied with the age and gain of the detector. Using the quoted resolution of 0.25mm for the detector, first order estimates tend to underestimate the image size to a value of 0.66mm , the simulation predicts 0.72mm but fits to Auger peaks indicate a width of 0.8mm .

Fig. 3 shows the in-plane response of the conical lens L2 as a function of the input parameters R, A and E for various values of r : the resulting matrix is given in eqn. (3). The axial magnification over this range can be varied from 0 to 5, as seen from Fig. 3a. The flatness of the line in Fig. 3b is an indication of the range and quality of the lens focus and the degree of aberration. The asymmetry of the lens also leads to small perturbations in the central orbit trajectory and a small dependence of the image position on incident energy, as shown in Fig. 3c and Fig. 3f.

Fig. 4 shows the characteristics of the Outer Toroid (OT) calculated for a pass energy of 1000eV . Two sets of curves have been drawn to illustrate the effect of applying a deflecting potential due to the IT set to a pass energy of 100eV . The OT resolving power is defined by eqns. (6) and (7). All the

Fig. 5. Inner analyser. Electron flight times to P4(MCP).
See text for explanation of (a) to (e).

Fig. 6. Outer Analyser. Electron flight times to P6(Outer toroid output).
See text for explanation of (a) to (e).

parameters, except C_R which is equal to $\partial R_{out}/\partial A_{in}$, are defined above. The various in-plane electron optical parameters have been calculated from Figs. 4a, 4b and 4c and are functions of the pass energy of the inner analyser. The values of the parameters are: $M_r(0)=1.06$, $M_r(100)=0.86$, $D_i(0)=0.113$, $D_i(100)=0.112$, $C_R(0)=-0.52$, $C_{R,A}(0)=-0.0015$, $C_R(100)=0.04$, $C_{R,A}(100)=-0.16$. The source width is approximately equal to the electron beam diameter w so $\Delta R_{in}=0.5\text{mm}$, ΔA_{in} is $1.17 \cdot (w/a_{out}) \cdot (180/\pi)$ and R_{det} is equal to $0.73 \cdot (\text{Output slit width})$. The resolving power of eqn. (7) is 116 without deflection and 132 with deflection. Experimental estimates from the transmission of elastically scattered electrons without deflection indicate an resolving power of approximately 120. Fig. 4d shows that the OT has an excellent angular resolution with an axial magnification M_H equal to 0.0089; the angular resolution is therefore principally dependent on the resolution of the detector at P6.

In summary, the field perturbation leads to a change in the pass energy of 4.8 eV which was experimentally verified by tuning an elastically scattered beam with and without deflection. Also, a change in the input angle of one degree and a reduced angular transmission in turn lead to an increase in the resolution of approximately 10% and an experimentally observed reduction in transmission also of around 10%.

Figures 5 and 6 indicate the electron flight times through the toroids as functions of the parameters input R , A , E , V and the output R . The important consideration is which contributions to the total flight time can be located and then compensated in software. The largest contribution of 1.35 nsec arises from the energy dispersion across the MCP which can be compensated, however the azimuthal angular contribution of 0.80 nsec causes little radial dispersion on the MCP and consequently cannot be compensated. The total timing resolution is 1.6 nsec and potentially could be 0.82 nsec for the conditions used.

The performance, particularly the angular response and the sensitivity, of the inner analyser, is indicated in Fig. 7. Fig. 7a shows the modelled results for a cross section which has a constant intensity for a series of discrete angles 22.5 degrees apart. The calculations were performed for three source sizes with standard deviations of 0.2, 0.5 and 0.8mm respectively, ie widths of 0.4, 1.0 and 1.6mm using the conventions of this paper. Unfortunately the angular width was found to vary with detection angle, the summed intensities are constant for all angles as expected. Fig. 7b shows measured angular intensities for emission of Auger electrons for a nominally isotropic distribution confirming the effect of source size. Fig. 7c compares the peak widths of Fig. 7a and Fig. 7b and indicates the real source has a standard deviation of 0.6mm diameter.

Also the well known elastic angular distribution [6] for scattering of 50 eV electrons from argon atoms was measured. This distribution has the distinctive features of a well defined, relatively narrow deep minima near 67° and 138° . A Monte Carlo intensity profile has been calculated for a finite Gaussian gas beam profile for nominal interaction cylindrical volumes with standard deviations from 0.1 to 1.5 mm. Fig. 7e shows the results of the calculated angular distribution with these intensity profiles folded into the standard cross section. Measured data were obtained using a long cylindrical tube with an exit diameter of 0.25 mm as the gas source located on the symmetry axis at a distance of 0.5 mm from the bottom of the electron beam with a width of approximately 0.5 mm. The gas pressure in the vacuum chamber during the measurements was 5×10^{-7} Torr. For these conditions the measured angular distributions are seen in Fig. 7d to be in excellent agreement with the standard data. The cut through Fig. 7e which gives best agreement corresponds to an interaction gas profile with a standard deviation of 0.6 mm which is in good agreement with the source size determined from the Auger peak and profiles obtained by scanning the electron beam through the gas jet.

The contributions from an extended source to the formation of the total image on the MCP are indicated in Fig. 8. In Fig. 8a the mid-grey annular region and the lighter grey oval region indicate the image shape using an isotropic cross section from a point source and from an extended source respectively. The lighter strips indicate the contributions of the scattering at 0° , 45° and 90° to the final image on the MCP. The reduction in the angular momentum of the particle causes a negative displacement in the radial plane which becomes significant for extended sources. The curvature is upwards due to the radial inversion from the lens.

Fig. 7. Modelled (open symbols) and measured (closed symbols) angular distributions for: (a) a source width of 0.2 $\circ$, 0.5 ∇ , and 0.8 $\square$ mm radiating at selected angles, also a summed intensity of each peak, (b) an angular cross section of a masked Ar Auger source, (c) the peak widths of (a) and (b) $\bullet$, (d) elastic scattering from Ar, 50 eV, source width 0.6 mm, (e) modelled elastic scattering from Ar, 50 eV, source widths 0 to 1.5 mm.

Fig. 8. The images formed by an extended cylindrical source and its subsequent removal from data: (a) the image at 0, 45, 90 degrees (b) the image of a continuous isotropic cross section (c) a cross section through (b) at 90 degrees for a central $\bullet$, 1.0mm displaced $\square$, and compact source — (d) subtraction of the central and displaced images (e) Ar L $\bullet$, M $\square$, M_{2,3} $\blacktriangle$ Auger peaks before and after subtraction of displaced image.

Fig. 8b shows the results of a Monte Carlo simulation of the radial (energy) profile image. The standard image shape for a compact 0.1mm source is symmetrical and sharply peaked as shown for the image at zero degrees. But for an extended 20mm long and 0.5mm diameter cylindrical source, from background gas emission, a highly asymmetric shape is found to extend to larger radii. This asymmetry stems from a range of emission angles contributing over the length of the source, illustrated in Fig. 8a for 3 discrete angles.

Fig. 8c compares angular cross sections for a series of simulations conducted with a centrally located point source, a centrally located, extended cylindrical source as described above and an extended cylindrical source laterally displaced 1mm. The angular cross sections have been integrated over an angular range of 30° to improve statistics and are centred at 90° to the electron beam. It is important to model this contribution accurately because in a dynamically pumped system with a flowing atomic beam, the background contribution rises as the beam density increases and must be subtracted from all angular distribution data.

One way of allowing for the contributions of the background scattering to the final image is suggested by Fig. 8c, that is to subtract the contributions from an image displaced laterally by a distance, ie 1 mm for example, which is outside the deduced diameter of the nominal source size. Displacement of the electron beam by 1 mm has been shown not to cause any discernible change in either the shape or position of the image. The residual intensity is shown in Fig. 8d, the intensities oscillate above and below zero due to poor statistics and as expected the technique is less effective near 0° and 180° . However the success of the method is evident and is confirmed by the data in Fig. 8(e). The $L_{2,3}M_{2,3}M_{2,3}$ Auger peaks of argon are shown before and after subtraction of the background in the above manner. The location of the peaks is unchanged, as they should be, while the widths are significantly reduced.

4. CONCLUSION

In conclusion the modelled characteristics are in good agreement with measured elastic and Auger peak widths, their relative intensities and angular distributions. The operating characteristics are straight forward for a small symmetric source of extent, say 0.3mm, which is less than 2% of the axial radius of the inner toroid. For the present toroid, the ratio of the image width to the axial radius of the toroid is typically 8% which was determined primarily by the size of an existing vacuum chamber rather than by fundamental principles determining the optimum analysis characteristics. For an extended source size, as would be characteristic of an in-plane crossed beam scattering experiment, it is essential to model the background gas contributions to the image. In that way state-of-the-art performance can be obtained.

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