Development of Spheroid Energy Analyzers for Elemental and Chemical Analysis of Surfaces

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Abstract

The spheroid energy analyzers (SEA) are a new class of charged particle energy analyzers that are characterized with very high energy resolution and transmission. The design of the first prototype analyzer is described. A novel geometrical framework is presented, that describes SEA analyzers in general terms within which the well known types of analyzers CMA and CHA appear to be only particular examples. A very high order of focusing of these analyzers is presented via simulation that indicates the existence of 13th order focusing in one of our models. Experimental results are presented showing relative energy resolution of 0.05 % of the pass energy at a transmission of 21 % out of a 2π steradian.

Keywords : Electron optics, Energy analyzer, Order of focusing, Auger electron spectroscopy, Photoelectron spectroscopy

1. Introduction

Charged particle energy analyzers are employed in various analytical instruments for elemental and chemical analysis of materials. The sample can be illuminated with X-rays, electrons or ions and electrons or secondary ions emanating from the sample can be energy analyzed giving rise to well established analysis techniques XPS, AES and ISS; X-ray photoelectron spectroscopy, Auger electron spectroscopy and Ion scattering spectroscopy, respectively. Among all different analyzers, described in numerous publications¹, the concentric hemispherical analyzer (CHA) and the cylindrical mirror analyzer (CMA) are the most common types. The geometry of these two analyzer types might be thought as to be very different; however, topologically their geometries are very similar. We describe a concept where geometries of both analyzers are just particular examples of a more general geometry that in turn provides numerous analyzer configurations, that we now call spheroid energy analyzers (SEA)², often having excellent electron optical characteristics. The SEA is a type of annular analyzer system. Unlike paraxial systems (like round lenses for example) annular systems make use of off-axis trajectories and the trajectories close to the axis are not used. The CMA is an example of annular system that is well known. Several general notes on annular systems can be found in Hawker's book in paragraph 42.6 where it was highlighted that some annular systems can provide high-order focusing. The SEA seems to be the first annular system that allows creation of numerous useful and annular systems can provide high-order focusing. The SEA is a type of annular analyzer system. Unlike paraxial systems (like round lenses for example) annular systems make use of off-axis trajectories and the trajectories close to the axis are not used. The CMA is an example of annular system that is well known. Several general notes on annular systems can be found in Hawker's book in paragraph 42.6 where it was highlighted that some annular systems can provide high-order focusing. The SEA seems to be the first annular system that allows creation of numerous useful and powerful analyzer embodiments. There have been sustained activities to modify the geometry of a CMA in order to achieve smaller aberration coefficient efficiencies and improve transmission; for example N. Kholine and Y. K. Golikov from St. Petersburg. Their model is described by solutions of the Laplace equation in cylindrical coordinates where radial and axial fi eld components are completely separated. A working prototype of this particular model has been demonstrated and published in Ref.4. The SEA differs from that particular model as the SEA fi eld is not the solution of the Laplace equation in the form of separated axial and radial fi eld components and also it differs as it represents a wide range of possible confi gurations. The SEA generalizes the CMA and CHA geometries and enables electron optical exploration of various new analyzer embodiments. A particularly interesting property of the SEA is high order focusing that in turn provides both high angular acceptance (transmission) as well as high energy resolution, simultaneously. In one practical embodiment of the SEA analyzer we have achieved transmission of 21 % out of 2π steradian and an energy resolution of better than 0.05 % at FWHM.

2. Analyzer construction

A schematic of the analyzer is shown in Fig. 1. The main electron optical elements of the analyzer are inner and outer electrodes. The electrodes are concentric and cylindrically symmetric with spheroid like shapes. Signifi cance of this electrode shape is described in more detail in paragraph 3. In our fi rst analyzer embodiment the inner electrode is made hollow and it accommodates a thermionic electron gun. The gun illuminates the sample with electrons and in turn electrons emanating from the sample entering the analyzer fi eld through the slit in the inner electrode are energy analyzed. This particular configuration enables AES, where electron energy spectra are recorded and the surfaces elemental composition can be worked out from characteristic energies of the Auger spectral lines. The analyzer’s inner and outer electrodes come close together at electrodes edges; hence this configuration does not require fringing fi eld correctors. This simplifies construction and voltage requirements. Photo-graphs of the main analyzer elements following assembly steps are shown in Fig. 2. The fi gure depicts (a) electron gun, (b) inner electrode, (c) outer electrode and (d) magnetic shield. The number of mechanical components has been minimized in order to provide better robustness and reliability of the analyzer. This analyzer embodiment fi ts 10" CF fi ane.
3. Analyzer geometry generalization

In pursuit of elegance and simplicity when describing the SEA fundamental geometry a novel analyzer geometry concept has been established that places different analyzer types within one geometrical framework.

To explain this we go back to the analyzer electrode shape. The main portion of the inner and outer electrodes shape of the SEA analyzer are created by rotating an ark of a circle of radius $R$ around an axis at distance $R_0$ in the meridian plane of the ark. The created 3D element is a spheroid like shape truncated at both ends. This is illustrated in Fig 3 (a) and (b).

Following this procedure a set of two spheroids can be created by selecting arks of two circles as shown in Fig. 3 (c). The two spheroids become parts of the inner and outer cylindrically symmetric elements of the SEA. Referring to Fig. 3 (c), we introduce dimensionless parameters $K$ to describe basic geometry features of the SEA analyzers. Three $K$ parameters are defined as

$$
K_1 = \frac{R_1}{R_{12}} \\
K_2 = \frac{R_2}{R_{12}} \\
K_3 = \frac{R_{02}}{R_{12}}
$$

(1)

Where $R_1$ and $R_2$ are radii of the two arcs of circles and where $R_{01}$ and $R_{02}$ are maximum distances of the respective arcs from the common longitudinal axis of rotation and where $R_{12} = R_{01} = R_{02}$, as it is depicted in Fig. 3 (c).

Using $K$ parameters the geometry of the CHA can be described by $K_1 = 1 + K_3$ and $K_2 = K_3$ because $R_1 = R_{01}$ and $R_2 = R_{02}$; while the CMA corresponds to $K_1 = K_3 = \infty$, coming from $R_1$ and $R_2$ effectively being infinite. Fig. 4 shows schematic of the CHA and CMA electrode shapes and corresponding geometry parameters.

![Fig. 1 Schematic of the SEA prototype with an internal electron gun](image1)

![Fig. 2 Main elements of the SEA prototype: (a) internal electron gun, (b) inner spheroid, (c) outer spheroid, and (d) magnetic shield](image2)

![Fig. 3 Illustration of the generation of the main electrode elements with relevant geometry labels](image3)

![Fig. 4 Towards unified description of CHA and CMA geometries](image4)
Any particular relation between the K parameters can be visualized by plotting them within the K coordinate system where three orthogonal axes are replaced with values of the three K parameters. In this novel coordinate system all the different CHA and CMA analyzers can be represented by a set of points on corresponding straight lines as shown in Fig. 5 (a). Moreover, various toroidal structures emerge if one enables concentric circular arcs with $R_1 \neq R_{01}$ and $R_2 \neq R_{02}$. All K values of such toroidal structures are on a single plane in the K coordinate system as shown in Fig. 5 (a).

All other different SEA geometry configurations, that we are particularly interested in, fill up an entire positive quadrant of the K space; this therefore generalizes the geometries of the several known types of analyzers, the most known among them being CHA and CMA.

Specifically the geometries of the SEA can be selected to satisfy $R_2 > R_1$ as depicted in Fig. 3 (c). This ensures that the truncated edges of the two spheroids converge towards each other rather than diverge away. Fig. 5 (b) shows the position of one such more narrowly defined region of the SEA geometries. Those configurations are selected as more practical because the converging edges of the spheroids enable very good truncation of the fringing fields between the two spheroids of the analyzer.

The described analyzer concept provides a range of hitherto unknown charged particle energy analyzers having spheroidal electrode surfaces. We refer to all of these as Spheroid Energy Analyzers. A prominent round point inside the SEA volume in Fig. 5 (b) represents K parameters $(K_1=2.756, K_2=4.889, K_3=0.944)$ of the prototype SEA embodiment that we have built in order to experimentally verify the SEA performance. The prototype is built with characteristic dimensions of: $R_1' = 124$ mm, $R_2' = 220$ mm, $R_{02}' = 42.5$ mm and $R_{12}' = 45$ mm. In practical embodiments of the SEA, the outer and inner elements of the analyzer are predominantly spheroids, but there could be disk, cylinder or cone like shapes. These are positioned at the edges of the main spheroids to truncate the field and achieve the desired mechanical shape. In the present embodiment, the inner element is typically kept at ground voltage while the voltage of the outer spheroid (element) is scanned to obtain the full spectrum. Charged particles are injected into the field through a slit in the inner element of the SEA and exit the analyzer through a second slit in that element.

![Fig. 5](image1.png)

(a) Representation of the CHA, CMA, and toroids geometry in the K coordinate system, (b) SEA region also marked in the K coordinate system

4. Analyzer electron optical properties

The electron optical characteristics of the SEA were obtained numerically via ray tracing within two charged particle optics programs; SIMION$^9$ and CPO$^6$. More detailed results of this first analysis were published previously$^7$ and only the main conclusions are listed here. Fig. 6 shows a model of the entrance of the analyzer with electron trajectories spanning angular range of 16° and showing working distance (WD), mid angle and the mid-point where the mid trajectory crosses into the analyzer dispersive field. We first examined focusing properties for the fixed mid-point by recording the axial position where the trajectory crosses the axis, so called ‘landing position’ as a function of entrance angle. Next, an n-th order polynomial is fitted to the landing position curve revealing order of focusing that by convention is n-1 of the first nonzero member of the polynomial.

![Fig. 6](image2.png)

Model of the SEA entrance region showing a representation of the inner electrode slit and a set of trajectories spanning the angular range of 16°

Fig. 7 Landing positions versus relative incident angle. Diamond shaped points: SEA simulation results for high order focusing. Full curve: the best least square fit n=14th order polynomial factor. Circles: SEA simulation results for low order focusing. Dashed curve: the best least square fit n=2nd order polynomial.

Fig. 7 shows the landing position curves for mid angle of 52° giving first order focusing and the landing position for mid angle of 47° degrees showing remarkable 13th order focusing. That the focusing is of a very high order is evident from the flatness of the focusing curve. Though the first order focusing in Fig. 7 (n=2 curve) is much inferior to the 13th order of focusing, it should be noticed that the total axial spread of the landing positions for n=2 is only about 250 µm. For comparison CHA of the same characteristic size and angular spread would produce a landing position trace that is about 5 mm long. Considering that the dispersions of the SEA and the CHA are similar this means that the SEA will deliver much higher energy resolution as the relative proportion of the pass energy that the CHA. About 40 times higher energy resolution is demonstrated in experiment as described in the next paragraph. This analysis is valid for a small source size at the entrance of the analyzer of roughly less than 50 µm wide in the dispersive direction of the analyzer.

The finite spot size in front of the analyzer influences energy resolution and becomes a dominant factor when the spot size is large. The energy resolution of various analyzer types becomes more similar. A differentiating factor in the case of the large entrance spot size becomes the transmission that preserves good spectral shapes. Fig. 8 shows Monte Carlo simulation of the 2D electron splat diagram and intensity profile at the detector plane for SEA and CHA obtained for 0.5 mm wide source and 13.7 ° half angle in both dispersive and non-dispersive directions of the analyzer. While SEA keeps the intensity profile symmetric CHA shows long tail that would deform spectral features if left unchecked. Consequently in practical applications CHA has to limit the angular spread in the dispersive direction of the analyzer to cut off the long tail. This in turn reduces transmission of the CHA typically by 60 % to 80 % with respect to SEA.

5. Experimental assessment of analyzer

The SEA performance is assessed within AES experiment. Fig. 9 shows the experimental configuration with an external electron gun with Schottky emitter. Fig. 9 (a) shows photograph of the front face of the SEA visible in the background and the front cone of the electron gun pointing towards the sample in the foreground. The SEA before assembly into the test chamber is shown in Fig. 9 (b). Fig. 9 (c) shows a secondary electron (SE) image of the sample area in front of the SEA obtained by scanning electron beam emanating from the external electron gun.

We determined the relative energy resolution of the SEA (\(\Delta E/E\)) experimentally by directly measuring the total FWHM of the backscattered electron peak, \(\Delta E_E\), from a clean stainless steel surface and by subtracting the width of the primary electron beam of the Schottky emitter, \(\Delta E_p\), in the usual quadratic manner: \(\Delta E^2=\Delta E_p^2+\Delta E_E^2\). The \(\Delta E_p=1\) eV is assumed. This method works properly when \(\Delta E_p^2<<\Delta E_E^2\) so a small uncertainty in the exact value of \(\Delta E_p\) does not influence the final result.

Fig. 10 shows a 5 keV backscattered elastic peak from stainless steel in the 4990-5010 eV energy interval. The analyzers relative energy resolution at FWHM was found to be \(\Delta E/E=0.048\%\). Fig. 11 shows another interesting example of the benefit of the SEA high intrinsic energy resolution and it compares SEA result with CMA and CHA. Here the backscattered spectrum of Germanium was measured at 5 keV incident beam energy. The high SEA energy resolution enabled clear observation of the main elastic peak as well as a series of less intense Plasmon losses spaced at characteristic 17eV intervals. A featureless solid curve in the diagram shows a simulated spectrum that a typical CMA instrument would obtain having relative energy resolution of 0.5 %. Moreover, Fig. 11 shows that the relative energy resolution as a percentage of pass energy of the CHA was 2 %. This in turn gave absolute energy resolution at FWHM of \(\Delta E=100\) eV which was 40 times larger than \(\Delta E=2.5\) eV obtained in the experiment with SEA.

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Dotted curve: Germanium backscattered spectrum at 5 keV incident energy obtained by SEA. Full curve: The same germanium spectrum convoluted with a Gaussian function of 0.5 % relative energy width. The CHA comparative energy resolution result is estimated.

Fig. 10  5 keV backscattered elastic peak from stainless steel

Tungsten and gold Auger spectra obtained by SEA. Both direct and numerically differentiated Auger spectra are shown along with zoomed in region with characteristic MNN Auger lines.

Fig. 11  Dotted curve: Germanium backscattered spectrum at 5 keV incident energy obtained by SEA. Full curve: The same germanium spectrum convoluted with a Gaussian function of 0.5 % relative energy width. The CHA comparative energy resolution result is estimated.

Fig. 12  Tungsten and gold Auger spectra obtained by SEA. Both direct and numerically differentiated Auger spectra are shown along with zoomed in region with characteristic MNN Auger lines.
6. Discussion

The SEA configuration experimentally examined in this work has confirmed the high resolution and high transmission properties found in simulations. Focusing in the plain containing the axis was discussed in this paper. The SEA can be configured also to focus away from the axis of the system. This results in a ring focusing that leaves the axis of the system free for other probes or excitation sources. The SEA can be combined with a position sensitive detector in which case 5 to 10% of the pass energy can be captured at the detector at once depending on desired energy resolution and transmission. The source of charged particles, described in this paper, was created by direct electron impact of electrons upon the sample placed in front of the analyzer. However, it is envisaged that the SEA can be coupled to other electron optical elements that in turn can form the source of charged particles acceptable by SEA.

7. Conclusion

A unified view of different analyzer geometries is presented. An insight into very high order of focusing energy analyzers is given. The approach presented here provides the possibility to realize analyzers that have both very high energy resolution and very high transmission. In the first constructed SEA prototype relative energy resolution at FWHM of 0.05% was demonstrated at transmission of 21% out of 2\pi steradians. We are on track to establish several more useful SEA configurations for analytical instrumentation in time to come.

References

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