Research Article

Simulation of Electron Energy Spectra of a Biased Paracentric Hemispherical Deflection Analyzer as a Function of Entry Bias: Effects of Misalignments

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The performance of a biased paracentric hemispherical deflection analyzer (HDA), including fringing fields and their effect on focusing and energy resolution, is investigated using numerical methods. Electron energy spectra are calculated for three entry positions $R_0 = 84$ mm, 100 mm, and 112 mm and compared with the recent experimental measurements. In both experiment and calculation, the two different paracentric entry positions $R_0 = 84$ mm and $R_0 = 112$ mm, on either side of the mean radius of 100 mm, are found to have a base energy resolution of about two times better than the conventional centric entry position $R_0 = 100$ mm. In order to explain the discrepancies (6–30%) between the simulated and the experimental resolutions the focusing characteristics are further investigated for different displacements of the input lens (ΔR_0) with respect to the entry position R_0 and the tilted input beam axis by α_{shift} in the dispersive direction. We have found that the blame does not in fact lie with the theory and we have shown that the input lens may have been misaligned in the experiment. Slight misalignments affect both the true energy resolution measurement and the transmission of the beam.

1. Introduction

The hemispherical deflection analyzer (HDA) combined with a cylindrical input lens system is the most often used electrostatic energy analyzer in very different fields of application including electron spectroscopy [1, 2], space science [3], mass spectrometry [4], coincidence spectroscopy [5], and electron microscopy [6]. The analyzer selects out ions or electrons with a particular kinetic energy and direction by successively readjusting the field of the analyzer allowing for higher transmission through small slits or apertures [7]. Like prism in light optics, the electrostatic energy analyzer (or filter) suffers from angular aberrations [8]. In particular, the elimination of aberrations caused by the inherent fringing fields at the boundaries of electrodes is of primary concern [9]. Fringing fields strongly perturb the ideal $1/r^2$ field at the entry and exit of HDAs, which is particularly severe if the gap between the hemispheres is made large ($\Delta R \equiv (R_2 - R_1) \geq 50$ mm) [10]. Departure from nonideal behavior drastically

deteriorates the first order focusing of the ideal HDA and hence reduces the energy resolution.

Many correction schemes have been developed in order to minimize the effect of fringing fields, for example, Herzog correction [11], Jost correction [12], tilted input beam axis [13], and concentric termination rings [14]. Apart from these, Zouros and coworkers [15–19] showed that the fringing field itself could also be used to restore first order focusing by simple displacement of the HDA entry R_0 from its conventional centric position (at the mean radius $R_m = (R_1 + R_2)/2$) to a new position with a nominal entry potential $V(R_0)$ without using any additional corrector electrodes. This is the result of the effective utilization of the intrinsic lensing properties of the fringing fields. This arrangement has been referred to as “biased paracentric” HDA. The exact position of these so-called paracentric positions were discovered using simulation and were found to be a function of the entry radius R_0 and the entry bias $V_0 = V(R_0)$ [19]. For a particular HDA geometry having a wide-gap interelectrode distance

$\Delta R = R_2 - R_1 = 50$ mm and a mean radius $R_m = 100$ mm and $R_0 = 84$ as well as $R_0 = 112$ mm were found through simulation to be the “magic” numbers. Recently measurements were made to test these findings in the electron-collision laboratory [20]. Experimental results showed the paracentric entries to lead to an improvement of about a factor of 2 over the centric position and close to the ideal HDA results. The discrepancy between experiment and theoretical calculation was within 20%–30% for the cases of $R_0 = 112$ mm and 100 mm and much larger than for the case of $R_0 = 84$ mm and therefore puzzling. It was concluded that such uncertainty was typical of mechanical tolerances in the construction of HDAs [21, 22].

The main objective of this work is to numerically analyze the biased paracentric HDA using ray-tracing calculations and examine some of the critical factors such as entry position, entry bias, and misalignments of the input lens (the entrance aperture) that affect both the true energy resolution measurement as well as the transmission of the beam. First, we calculate the characteristic features of the analyzer such as dispersion, transmission, and focusing for three entry positions, $R_0 = 84, 100$, and 112 mm. Second, simulated electron energy spectra and energy resolution are compared with the experimental measurements. The results of numerical simulations of spatial profiles of the misaligned beam are presented.

2. Materials and Methods

2.1. Analyzer Voltages. The details of the electron optical properties of HDAs are well described in the literature [18, 23–25], so we will only give a brief overview of the HDA here. A typical HDA consists of two coaxial hemispherical electrodes held at different potentials and an electrostatic input lens. There is a small entrance (and exit) aperture through which electrons are accepted. From the analysis of trajectory equations, the potentials of the inner and outer hemisphere satisfy the following equation for an electron of kinetic energy E_0 passing through the HDA:

$$qV_i = E_0 \left\{ 1 - \frac{\gamma}{\xi} \left[\frac{R_0(1 + \xi)}{R_i} - 1 \right] \right\} \quad (i = 1, 2), \quad (1)$$

where R_1 and R_2 are the radii of the concentric inner and outer hemispheres, respectively, and R_0 is the beam entry position. The voltages on the hemispheres V_1 and V_2 are adjusted so that an electron entering the analyzer at R_0 with an energy E_0 and angle $\alpha = 0$ exits the analyzer at $R_\pi = (R_1 + R_2)/2$. This E_0 is called “the pass energy” and the trajectory the *central ray*. ξ is the HDA *paracentricity* defined as $\xi = R_\pi/R_0$, while γ is the *entry biasing parameter* defined as $\gamma = 1 - qV(R_0)/E_0$. $V(R_0)$ is the nominal potential at the entry at R_0 , which corresponds to the image position of the input lens. Thus, a conventional centric HDA is a special case of the biased paracentric HDA with $\xi = 1$ and $\gamma = 1$.

2.2. Electron Optical Properties. If an electron enters this analyzer at $r_0 = R_0 \pm \Delta r_0/2$ with an energy $E = E_0 \pm \Delta E/2$ and at small angles, then the electron will leave the analyzer

at $r_\pi = R_\pi \pm \Delta r_\pi/2$. Under these conditions, the exit beam trace width Δr_π is given by [26]

$$\Delta r_\pi = |M| \Delta r_0 + D \frac{\Delta E}{E} + P_1 \alpha_{\max} + P_2 \alpha_{\max}^2. \quad (2)$$

Here, the first term shows the magnification (M), the second energy dispersion (D), and the third and last terms first- and second-order angular aberration coefficients (P_1 and P_2 , resp.). The angle $\alpha_{\max}$ is the maximum half angle at the entrance of the HDA permitted by the input lens. By neglecting the fringe field effects at the entrance and exit of the HDA, one can obtain that $M = -1$, $D = (1 + \xi)R_\pi/\gamma$, $P_1 = 0$, and $P_2 = -D$. $P_1 = 0$ means that the ideal HDA has first-order angle focusing [27]. It should be noted that two HDAs in series can compensate for the second-order angular aberration ($P_1 = 0$ and $P_2 = 0$) if the field in the two HDAs is adjusted properly [6]. For a monoenergetic point source ($\Delta E = 0$ and $\Delta r_0 = 0$), the dispersion of the ideal centric HDA is $2R_0$, and the ratio of trace width to dispersion is $\alpha_{\max}^2$ [28]. Note that the energy resolution is directly related to dispersion feature (chromatic aberration) of the analyzer. For the centric conventional ideal HDA, the energy analysis described by (2) with a dispersion $D = 2R_0$ results in a band pass with a base width of ΔE_B which is given by the well-known resolution formula:

$$\frac{\Delta E_B}{E_0} = \frac{(w_1 + w_2)}{2R_0} + \alpha_{\max}^2, \quad (3)$$

where w_1 and w_2 are the HDA entrance and exit slit width along the dispersion direction. The base energy resolution $\Delta E_B/E_0$ is determined both by the entrance and exit width and the acceptance angle [29]. Improvement in resolution can be obtained using decelerating input lens (lowering pass energy) at the cost of worsening transmission or by increasing the mean radius which increases the overall dimension and pumping requirements [8].

The purpose of the decelerating input lens system is to reduce the electron energy E_s to E_0 while maintaining total transmission. We may define $F = E_s/E_0$, the ratio of the particle energy at the object side to that at the image side. Then, the overall energy resolution of a hemispherical deflector may be described by the equation

$$\frac{\Delta E_B}{E_s} = \frac{\Delta E_B}{E_0} \frac{E_0}{E_s} = \left(\frac{\Delta r_\pi}{D_\gamma} \right) \frac{1}{F}. \quad (4)$$

The energy dispersion D_γ and the trace width Δr_π are two common terms that measure the quality of the analyzer. The decelerating input lens has to be designed with special attention to the problem of optimizing the spectrometer resolution [30].

2.3. Simulation Details. A series of computer simulations has been performed for the paracentric HDAs (without the lens) and the figures of merit: energy resolution and image properties are then computed in terms of source position, analyzer angular acceptance, and initial kinetic energy distribution. Since the equation of motion of

FIGURE 1: A visual representation of the focusing capability, the image size, and dispersion at the detector produced by two bundles of electrons formed by 100,000 inputs, in which the particle initial conditions are generated by a random process with two pass energies $E_0 = 50$ eV and $E' = 50.8$ eV, and $\alpha_{\max} = 5^\circ$ for an extended source of $\Delta r_0 = 2$ mm and for (a) $R_0 = 84$ mm, (b) $R_0 = 100$ mm, and (c) $R_0 = 112$ mm, respectively. A hemispherical deflection analyzer creates a focus in both dispersive (y -axis) and nondispersive (z -axis) directions. A large dispersion and small trace width increase energy resolution.

an electron in a fringing electrostatic field cannot be resolved analytically, the focusing properties have to be determined by a ray-tracing procedure. We used the commercial particle trajectory analysis software SIMION v8.0 to obtain all field and trajectory solutions. The scaling used in the simulations was 10 grid units per mm (gu/mm) for better accuracy [31]. The scale and geometry of the analyzer are directly based on the experimental specifications given by [20]. Briefly, the simulated HDA consists of two concentric hemispherical surfaces with radii of R_1 (75 mm) and R_2 (125 mm). The analyzer was modeled for the case of equal width entrance and exit apertures ($w_1 = w_2 = 2$ mm). Three entry positions were studied: $R_0 = 84$ mm, 100 mm, and 112 mm. The correct voltages V_1 and V_2 have been set according to the formulas given in (1). In all of the calculations described here the energy of the electrons in the electron source was set at $E_s = 200$ eV ($\Delta E_s \sim 0.7$ eV). Calculations were then carried out to obtain the peak structure of electrons for a pass energy of $E_0 = 50$ eV, so the deceleration factor $F = 4$. The electron beam originated as a cone distribution, with a maximum half

angle of 5° at the HDA entry, in which case the ratio of the angular term ($\alpha_{\max}^2$) to the “slit term” ($(w_1 + w_2)/2R_0$) is lower than 0.5, which fulfills the Kuyatt-Simpson criterion [32]. Once the simulation is complete, the electrons are sorted into equally distributed position bins to determine the transmitted electron spectra for a given position. The maximal difference between the various exit radial positions r_π defined the radial trace width Δr_π . This was directly converted into the energy width ΔE_B by an energy calibration procedure [19]. The determination of Δr_π and its corresponding ΔE_B was carried out in this way for each R_0 .

3. Results and Discussion

3.1. Focusing and Dispersion. In order to calculate the spatial and energy spread of the electron beam, simulations at two different pass energies of 50 eV and 50.8 eV have been performed as a function of the biasing parameter γ for three entry positions $R_0 = 84$, 100, and 112 mm, respectively. Figure 1 illustrates a sample set of electron trajectories that

FIGURE 2: Experimental [20] (circles) and computed (solid lines) energy spectra showing at three different values of the entry position R_0 : (a) 84 mm, (b) 100 mm, and (c) 112 mm. The analyzer was set to pass the electrons with a kinetic energy of 50 eV.

are emitted from the HDA entry and successfully reach the HDA exit (detector), thus illustrating the energy dispersion of the analyzer. To represent all possible trajectories, $N_e = 100,000$ electrons are emitted from a finite source (area: $4\pi \text{ mm}^2$), and their velocity vectors are randomly distributed. Here, the y -axis is the dispersive direction and the z -axis the nondispersive direction. One can verify the size and the shape of the image as compared to that of the finite source. Since the trace width and dispersion are directly related to the energy resolution, the best energy resolution can be achieved at $\gamma \approx 0.6$ for $R_0 = 112 \text{ mm}$ and $\gamma \approx 1.5$ for $R_0 = 84 \text{ mm}$. The simulation results for the central entry $R_0 = 100 \text{ mm}$ show that focusing effect becomes poorer (angular aberrations are quite high) and the electrons have a diverging trend which may lead to the increase of the trace width. Moreover, the peak positions for $R_0 = 100 \text{ mm}$ stay fixed as the biasing parameter is varied. However, for two paracentric entries the peak positions are shifted. Therefore, an extra energy calibration is needed for paracentric entry HDAs.

3.2. Comparison of Energy Spectra. The simulation was conducted with the biased paracentric HDA in order to compare the experimental and simulated electron loss spectra for three entry positions. The results are shown in Figure 2, in which the measurements are shown as circles and the calculations as solid lines. It is clear that the agreement between experimental and simulated spectra for $R_0 = 112$ is quite good, but for $R_0 = 100 \text{ mm}$ and, especially, for $R_0 = 84 \text{ mm}$ simulated spectra differed by more than 30%. Many calculations for different energy and angular distributions were repeated, but they reached the same conclusion. On the other hand, the strange multiple peak structure observed in the experiment shown in Figure 2(a) for $\gamma = 1.0$ and $\gamma = 1.2$ was not observed in the simulation.

The alignment of the HDA with the input lens is a critical experimental procedure. In the experiment, the input lens was aligned to the HDA entry by visual inspection and the correctness of the alignment was tested for only $R_0 = 100 \text{ mm}$ by using a HeNe laser which was mounted to a viewport of

FIGURE 3: Computer-simulated images of the electrons on the detector obtained with $E_0 = 50$ eV for $R_0 = 84$ mm and $\gamma = 1.8$ and for different values of ΔR_0 indicated above each column and α_{shift} indicated near each row.

the vacuum chamber as usually done. The laser and the analyzer were positioned such that the laser light entered the analyzer through the lens end and exited through the hole on the back of the hemispheres for $R_0 = 100$ mm. For other paracentric entries, misalignments as well as positioning errors are not known precisely enough. When the misalignment of the input lens occurs, the theory and optimal γ value no longer match the experiment. An example can be seen in [21]. It has been previously shown that the optimal γ was sensitive to a small change in R_0 [17]. So, our concern is the effect of misalignment on the energy resolution, particularly when the input lens is located at $R_0 = 84$ mm.

The input lens misalignments are implemented by means of displacements of the input lens such that its axis crosses the entrance plane of the HDA at the entry point ($R_0 \pm \Delta R_0$) and its direction deviates from the nominal lens optical axis by small angles (α_{shift} , β_{shift}) defined in the dispersive and nondispersive directions, respectively. The symmetry feature of the analyzer allows us to ignore the possible effect of β_{shift} and so we concentrate on the situations when $\beta_{\text{shift}} = 0$ and the misalignment in the entry position, ΔR_0 , along the dispersive direction.

Figure 3 illustrates simulated patterns of the beam intensity profiles obtained with $E_0 = 50$ eV for different values of ΔR_0 and α_{shift} for $R_0 = 84$ mm and $\gamma = 1.8$, in which the discrepancy between experiment and simulation is clearly seen (see Figure 2(a), 1st column). In case of no misalignment (the image at the center), the beam is distorted in the dispersive direction: the expected circular beam is

replaced by an asymmetric beam. This happens because $\gamma = 1.8$ is not an optimal value if there is no misalignment ($\Delta R_0 = 0$ mm and $\alpha_{\text{shift}} = 0^\circ$). However, the experimental results indicate that it gives the smallest spot size. It is seen that the lens misalignments produce changes in the spatial profile of the resulting beam. Comparing the patterns for $\gamma = 1.8$, one can conclude that increasing ΔR_0 from 0 up to 2 mm and α_{shift} from 0° to $+2^\circ$ makes practical influence on the spatial profile of the beam. Slight misalignments of the input lens in the analyzer could cause the shift of optimal γ value from 1.5 to 1.8. This fact inspires an interesting consequence: changing the entry bias eliminates the problem of angular and positional misalignments.

In Figure 4, we compare the simulated (solid lines) and experimental (circles) energy spectra for $R_0 = 84$ mm with and without misalignments. In the absence of any misalignment (Figure 4(a)), the resulting line shape loses its symmetry with increasing γ . As it is seen in Figure 4(c), taking $\Delta R_0 = +2$ mm and $\alpha_{\text{shift}} = +3^\circ$, the energy spectra appear to be symmetrical with further increase in γ , and the simulated spectra are in good agreement with the experimental ones. Other possibilities also occur, for example, $\Delta R_0 = +5$ mm and $\alpha_{\text{shift}} = 0^\circ$, but a misalignment in the entry position of 5 mm is difficult to assume.

3.3. Energy Resolution. Initial energy (ΔE_0), spatial (Δr_0), and angular (α_{max}) distributions of the beam affect the energy resolution of the analyzer. The measured and calculated base energy resolutions $\Delta E_B/E_s$ are plotted as a function of

FIGURE 4: Experimental [20] (circles) and computed (lines) energy spectra showing at $R_0 = 84$ mm with (a) $\Delta R_0 = 0$, $\alpha_{\text{shift}} = 0^\circ$, (b) $\Delta R_0 = 2$ mm, $\alpha_{\text{shift}} = 0^\circ$, and (c) $\Delta R_0 = 2$ mm, $\alpha_{\text{shift}} = 3^\circ$, respectively.

the biasing parameter γ for three entry positions in Figure 5. Experimentally, the width of the elastic scattering peak is defined by the temperature of the filament of the electron gun and the analyzer parameters. After convolution of the gun resolution from both the experimental and computed spectra, we obtained the base energy resolution. The resolution is shown as the base width and not as the full width at half maximum (FWHM). Here, the lines are the simulation results and the symbols with error bars are the experimental results [20]. It can be seen that the experimental data in Figure 5(d) are well reproduced by the theoretical predictions when the experimental misalignments are taken into account. In this case, a minimum occurred at $\gamma \approx 1.8$ for $R_0 = 84$ mm and $\gamma \approx 0.6$ for $R_0 = 112$ mm.

The main differences between our calculation and [20] are that they used a monoenergetic ($\Delta E_0 = 0$) angular electron distribution and a virtual aperture size, and the values of Δr_0 and α_{max} are controlled by the linear and angular magnifications of the lens. However, in the present work, the line shape simulations used a Monte Carlo approach in which both entry position r_0 and launching angle α were randomly sampled independently over the values $R_0 - \Delta r_0/2 \leq r_0 \leq R_0 + \Delta r_0/2$ and $|\alpha| \leq \alpha_{\text{max}} = 5^\circ$, assuming uniform illumination of the entry aperture region $\Delta r_0 = 2$ mm for a pass energy of

$E_0 = 50$ eV assuming a Gaussian distribution of $\Delta E_0 = 0.7$ eV (FWHM).

4. Conclusions

Using computer simulation, we have investigated the characteristic features of the biased paracentric HDA for different values of the entry biasing parameter γ at the three entry positions $R_0 = 84$ mm, 100 mm, and 112 mm and compared the theoretical predictions with experimental results reported in [20]. Overall, the two biased paracentric entry configurations showed good focusing characteristics and were found to be superior to the conventional centric HDA. We have also analyzed numerically the consequences of misalignments of the input lens, especially for the case of $R_0 = 84$ mm. For $R_0 = 100$ mm and 112 mm, simulation and experiment are consistent within an experimental uncertainty, and a small deviation of about 6% of the calculated energy spectra from that measured experimentally is observed. However, the maximum deviation is about 30% as found in the case of $R_0 = 84$ mm.

In the biased paracentric HDA, the input lens axis should be orthogonal to the entrance plane, and it crosses this plane exactly at a predefined entry position R_0 . Small positional

FIGURE 5: Dependence of energy resolution on the biasing parameter γ . Lines are the simulation results and symbols with error bars are the experimental results [20].

and angular deviations of the input lens lead to obvious geometrical transformations of the output beam profile. It was found that the discrepancy between experiment and simulation might have been due to the misalignments of the input lens. Additionally, we have shown that the entry biasing parameter γ can be used for controlling the effect of misalignments. Such misalignments are inevitable in real HDAs and the knowledge concerning their influences is, therefore, helpful for designing and arranging the fringing field correction schemes.

Finally, from the experimental point of view, there need to be more scientific approaches in testing biased paracentric HDA. In the spectrometer setup used to test this analyzer, each time the entry position R_0 is changed, it is necessary to open the vacuum chamber and insert a new electron source. Of course, this is time consuming and the experimental parameters such as the heat of the filament and target gas pressure were not identical from one experiment to

the other. A more sophisticated approach can be devised for the paracentric HDA so that the position of R_0 can be effectively varied without breaking vacuum. In addition, the energy distribution of the electron source should be minimized by using an electron monochromator or autoionization peaks of noble gases can be recorded instead of the elastic peaks.

Conflict of Interests

The author declares that there is no conflict of interests regarding the publication of this paper.

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