Experimental energy resolution of a paracentric hemispherical deflector analyzer for different entry positions and bias simulated in SIMION

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Abstract

Results from the simulation of a biased paracentric hemispherical deflector analyzer (HDA) with injection lens are presented. The finite differences electron optics software SIMION was used to perform Monte Carlo type trajectory simulations in an effort to investigate the focusing effects of the HDA entry and exit fringing fields which are used to improve energy resolution - a novel feature of this type of analyzer. Comparisons to recent experimental results are also presented. Biased paracentric HDAs represent a novel class of HDAs, which use the lensing action of the strong fringing fields at the HDA entry, to restore the first order focus characteristics of ideal HDAs in a controlled way. The improvement in energy resolution and transmission without the use of any additional fringing field correction electrodes is of particular interest to modern analyzers using position sensitive detectors.

Keywords: Hemispherical Analyser, Electron Spectroscopy, SIMION, Electromagnetic Lens

1. Electrostatic Analyzers & Experimental Setup

Electrostatic energy analysers are irreplaceable as high-resolution monochromators and energy spectrometers of ions and electrons in various atomic collision experiments, as well as in almost every experimental set-up for surface characterization. In general, a Hemispherical Detector Analyser (HDA) combined with a cylindrical input-lens-system is used to measure the energy of the scattered electrons in collision experiments.

The present analyzer uses a wide gap interelectrode distance ΔR=50mm and a mean radius of 100mm. It incorporates a standard input 5-element lens, which in this case is mounted on a rail to allow for the repositioning at the two paracentric entry positions $R_0 = 84$ mm and $R_0 = 112$ mm, compared to $R_0 = 100$ mm (the conventional mean entry). The complete HDA and 5-element lens as it was used in the laboratory is shown in Fig: 1.

Over the last decade it has been shown in simulation[1], that larger aberrations produced at the dispersion plane by fringing fields which tend to deteriorate the energy resolution of the analyser[2], can be readily overcome with such a "biased paracentric" HDA[3]
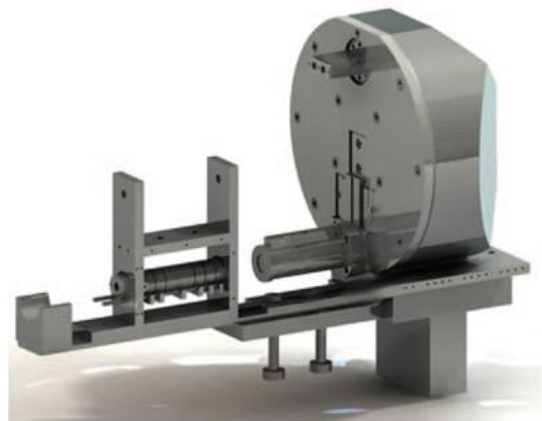

Figure 1: The actual setup of the analyser in 3D. The HDA and movable lens are enclosed in an insulated shell. In front of the lens is the electron gun.

2. SIMION Simulations

SIMION v.8.1 software package[4] was primarily used to calculate the electric fields and the trajectories of the flying particle. The first part of the simulation process was to design accurately and effectively the whole system (HDA and 5-element lens) so as to represent as precisely as possible the real analyser. For this we designed the analyser inside SIMION using the programming language LUA. It seemed that the resolution of the design (in milimiters per grid units) played a major role on the accuracy of the trajectories, so we used a fairly small grid size density of 0.5 mm/gu for an apparatus covering a near cubic volume of more than 300 mm extend on each side and that was the best possible resolution we could achieve utilizing all RAM. A complete 3D design of the HDA and 5-element lens is shown in Fig: 2.

The Laplace equation was later solved for every grid unit (gu) (an action called "Refine" in SIMION) and the design was imported into the workbench (as shown in Fig: 3) in a single 3D potential array (known as "instance" inside SIMION) where the variables such as number and position of particles, voltages of the electrodes and initial energies were defined for the simulation to take action.
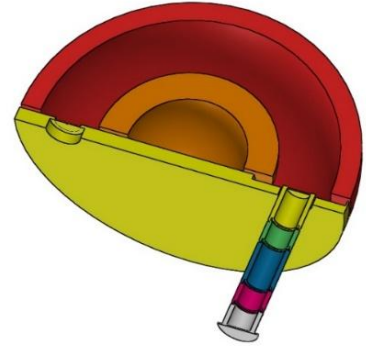

Figure 2: The 3D model of the HDA and 5-element lens, as it was designed inside SIMION. Each color denotes a different potential
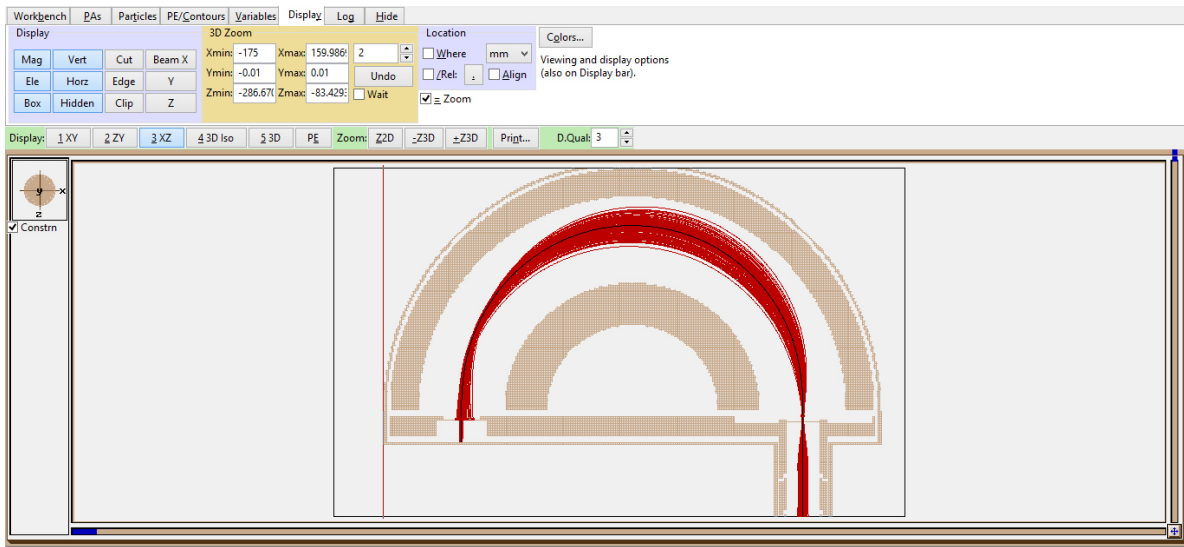

Figure 3: The SIMION workbench where all variables can be adjusted so at to start flying the particles. Automation coding is also supported, which can save a significant amount of time by running multiple simulation conditions at once.

3. Results

The performance of the analyzer was tested by energy analyzing the elastic electron-scattering peak for different γ values of the entry bias at the three entry positions, $R_0 = 100$ mm, 84 mm, and 112 mm, respectively. Two different simulation approaches were used in which the same 2D monoenergetic angular electron distribution was used for consistency. For each of the three values of R_0, the lens voltages were set fixed and HDA voltages were set depending on both variables R_0 and γ.

The first simulation approach, termed the "beam width" method, was based on determining the maximal beam width $\Delta r_{\pi max}$ and dispersion D_γ. $\Delta r_{\pi max}$ measured the maximum beam width along the dispersion direction (x-axis) on the plane of the exit aperture. D_γ was evaluated for each γ by "flying" a set of different energy E_i trajectories with $\alpha = 0$ and recording their exit positions r_π. After a few calculations we could obtain the base energy resolution which is shown in Fig:4 as the blue line.

The second approach termed the "voltage scan" method was obtained by stepping the voltages of the HDA and recording the number of electron trajectories that go through the exit aperture for each step. During the scanning of the voltages the pass energy of the electrons was fixed at 50 eV. The voltages were stepped in 0.1 or 0.2 eV steps so as to cover the entire electron peak. The base energy ΔE_B of the line profile could be directly determined from the final energy spectrum and was used to compute the overall base resolution R_{Bs0}. These results are shown in Fig:4 as the dotted green line.
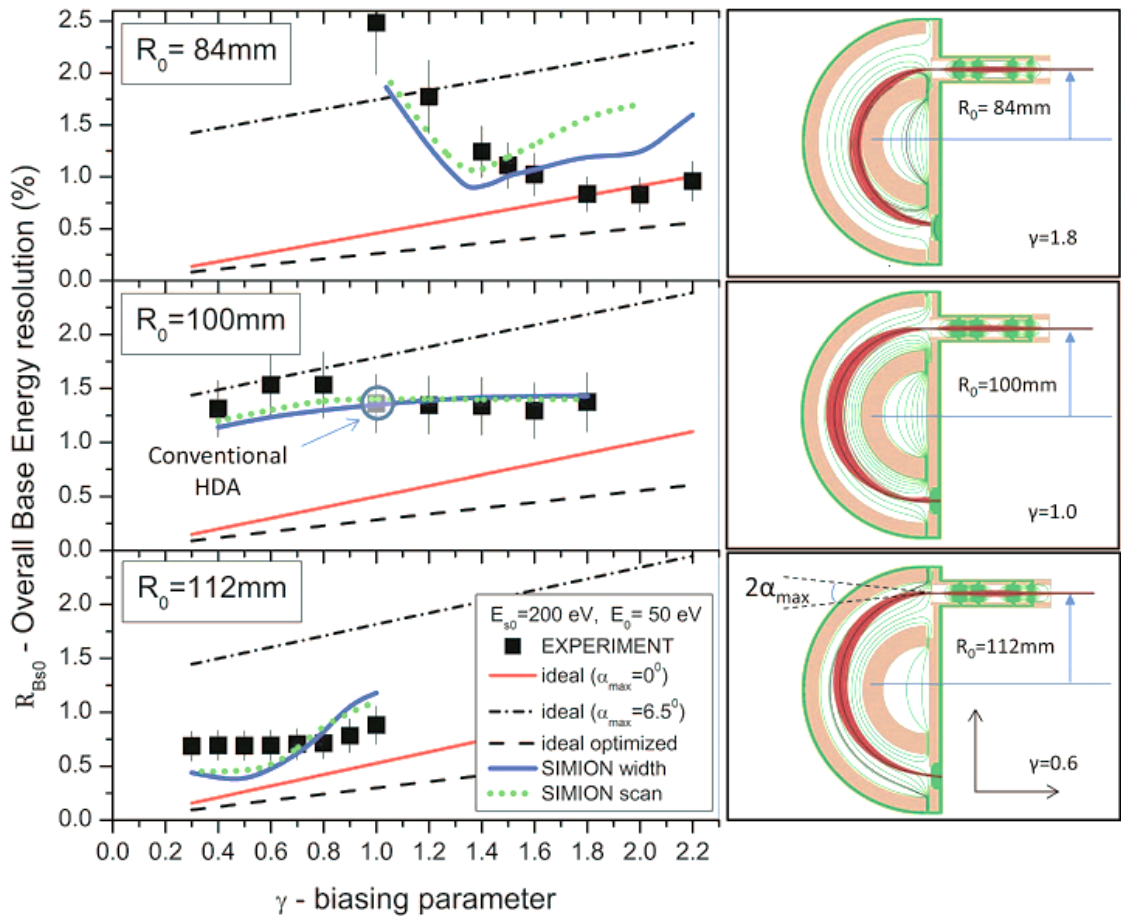

Figure 4: (Left) HDA overall base resolution R_{Bs0} plotted as a function of the biasing parameter for experimental, simulation and theoretical calculations for the 3 positions of the lens. (Right) Respectively, the schematics of SIMION simulations in the Y=0 dispersion plane of the spectrometer for conventional and paracentric positions. Electron trajectories are shown in red and equipotentials in green.

With the exception of the cases of $R_0 = 84$ mm with $\gamma > 1.5$ good overall consistency was found[5] between the two approaches which usually differed by less than $\sim 15\%$ for most points evaluated. The resolution for the (conventional) entry at the mean radius $R_0 = 100$ mm was found to be 1.6-2 times worse than the resolution for the two (paracentric) positions $R_0 = 84$ and 112 mm at particular values of the bias $V(R_0)$.

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Acknowledgments

References

[1] T. J. M. Zouros, O. Sise, M. Ulu and M. Dogan, Using the fringing fields of a hemispherical spectrograph to improve its energy resolution, Meas. Sci.Technol. **17**, N81N86, (2006)

[2] T. J. M. Zouros and E. P. Benis, J. Electron Spectrosc. Relat. Phenom. **125, 221248** (2002); "Erratum", **142, 175** (2005)

[3] O. Sise, G. Martinez, T. J. M. Zouros, M. Ulu, and M. Dogan, J. Electron Spectrosc. Relat. Phenom. 177, 4251 (2010)

[4] SIMION version 8.1.1.29, 12/29/2012, Scientific Instrument Services, Inc.,Ringoes, NJ, see http://www.simion.com .

[5] Dogan, M. Ulu, G. G. Gennarakis, and T. J. M. Zouros, Experimental energy resolution of a paracentric hemispherical deflector analyzer for different entry positions and bias, Rev. Sci. Instrum. **84**, 043105 (2013)