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The voltage optimization of a four-element lens used on a hemispherical spectrograph with virtual entry for highest energy resolution

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ABSTRACT

The methodology and results of a detailed four-element lens optimization analysis based on electron trajectory numerical simulations are presented for a hemispherical deflector analyzer (HDA), whose entry aperture size is determined by the injection lens itself and is therefore virtual. Trajectory calculations were performed using both the boundary-element method (BEM) and the finite-difference method (FDM) and results from these two different approaches were benchmarked against each other, to probe and confirm the accuracy of our results. Since the first and last electrode are held at fixed potentials, the two intermediate adjustable lens electrode voltages were varied over the entire available voltage space in a direct, systematic, brute-force approach, while minima in beam spot size on the 2-D position sensitive detector (PSD) at the exit of the HDA were investigated using a beam shaping approach. Lens voltages demonstrating improved energy resolution for the combined lens/HDA/PSD spectrograph system were sought with and without pre-retardation. The optimal voltages were then tested experimentally on the modeled HDA system using a hot-wire electron gun. The measured energy resolution was found to be in good overall agreement with our simulations, particularly at the highest resolution (~0.05%) working conditions. These simulations also provide a detailed insight to the distinctive trajectory optics and positions of the first and second image planes, when the PSD has to be placed some distance away from the HDA exit plane, and is therefore not at the ideal optics conjugate image position. The substantial time savings afforded over usual trial-and-error experimentation should make this type of make-do simulation approach attractive to experimentalists.

1. Introduction

Electrostatic cylindrical lenses are widely used to control beams of charged particles with various energies and directions in experiments covering many fields of applications including electron spectroscopy, surface science and mass spectrometry. It is well known that multi-element lenses are very useful in electron-optical systems due to their exceptional focusing capabilities (see, for example, Ref. [1] and references therein). In particular, the combination of a multi-element cylindrical lens with a hemispherical deflector analyzer (HDA) and a position sensitive detector (PSD) [2–6] has led to the development of technologically advanced and widely-used high resolution electron spectrographs (for a recent review see Ref. [7] and references therein), found in top research facilities around the world including synchrotrons [8], femtosecond lasers [9], Free Electron Lasers (FELs) [10], highly-charged ion sources [11] and heavy ion accelerators [12] enjoying high throughput with unprecedented energy resolution. It is also successfully marketed by many companies.

Typically, these lenses use *four* or more cylindrical electrodes in order to provide both focusing and pre-retardation of electrons to improve performance. Their performance has been investigated

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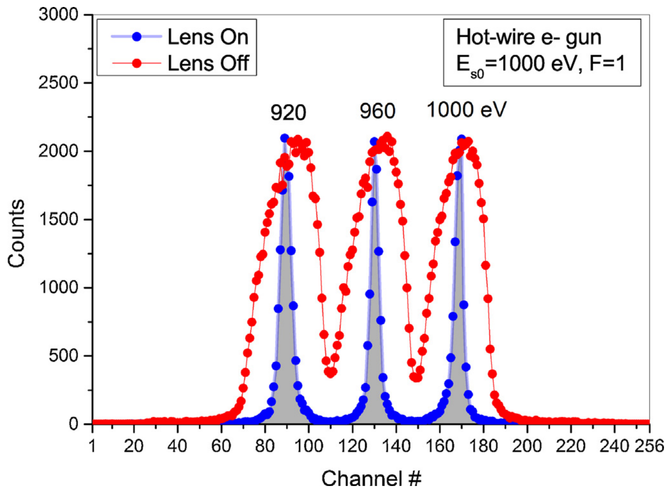

Fig. 1. Energy spectrum produced by a hot-wire e-gun recorded on our spectrograph without pre-retardation (F = 1). Line profiles for the injection lens on (Set 3 voltages – Table 3) or off (all lens electrode voltages zero, i.e. $V_{L4} = V_{L5} = 0$) are shown as detected along the HDA dispersion direction on the PSD. The importance of the lens on the energy resolution of the spectrograph is clearly shown for the *virtual* HDA entry investigated in this work. Here, the physical size of the HDA entry aperture d_a = 6 mm is very large, but with optimized lens focusing, the electron beam's HDA entry diameter can be made close to 10 times smaller, tantamount to an effective *virtual* HDA entry aperture of this size. For spectrometers with very small *real* entry apertures (e.g. $d_a \lesssim 0.5$ mm), the lens primarily affects the overall transmission and not the resolution, in this case mostly determined by the physical size of the real HDA entry aperture [14].

mostly in *isolation* from the HDA they usually serve since, under *ideal* conditions, they have to image the source onto the well specified position of the HDA entry plane. Thus, their performance has been extensively investigated mostly in terms of providing the smallest chromatic and angular aberrations [1,2] which works well for slit or aperture type HDAs. In these HDAs the size of their entry and exit slits/apertures primarily determines their energy resolution and the lens' goal is primarily to provide the highest possible transmission with minimum angular aberrations, thus ensuring near optimal operation.

However, when PSDs are used instead of exit slits/apertures, as in the more modern spectrographs, due primarily to space limitations at the HDA exit, it is rarely possible – if ever – to place the detector surface exactly at the HDA exit plane as required by the *ideal* HDA *first-order* focusing conditions. Instead, the PSD can only be placed a distance h away from the exit plane and outside the HDA, with h value varying between 15 and 25 mm. Typically, the smallest possible h is used in an effort to get as close as possible to the ideal conditions. Thus, choosing the optimal voltages for an injection lens on such a spectrograph with $h > 0$ is not straightforward. For many companies selling such expensive systems this is considered proprietary information obtained mostly by tedious experimentation.

In fact, the optimization of such an injection lens cannot be performed any more in isolation from the HDA and PSD, requiring instead a new approach where the investigation of the lens properties must be done *in situ* together with the rest of the spectrograph. This is even so for the case, when there is no *real* defining HDA entry aperture, but a *virtual* entry is used instead – strictly defined by the dimensions of the lens image – which may be well inside the field of the HDA itself [13], further exacerbating the lens optimization procedures. An example of the importance of such a lens with a virtual entry HDA is shown in Fig. 1.

In this report, we present the first to our knowledge such investigation using simulations to study the entire lens, HDA and PSD system together (we shall refer to this as the spectrograph) for conditions leading to the best energy resolution. We study such a spectrograph in simulation using a four-element injection lens which has only two independent lens voltages that need to be determined. Our optimization, in a brute force approach evaluates a representative sample of electron trajectories over the *complete voltage space* available to the two lens electrode voltages, thus in principle finding the *global* minima in the energy resolution of the spectrograph as extracted from the 2-D image recorded on the PSD itself. Our numerical approach thus extends existing simulations of HDAs with slits/apertures and single channel detectors [15] to more modern multi-channel detection HDAs.

As a final test of our approach we compare our results to experimental measurements on our real spectrograph (a paracentric HDA with 2-D PSD [12,16,17]). Some preliminary results have already been presented in various conference proceedings [18,19]. Two numerical simulation methods, the FDM and BEM, were employed in our optimization investigation [20]. The differences in the final *absolute* positions on the PSD of the integrated trajectories by both methods were within 0.8% or less, while differences in beam spot size were less than 0.15%, assuring the precise modeling of the experimental setup. The success of our approach is judged on two levels: (a) that it provides as good or better energy resolution than lens voltages previously used and discovered via *empirical* tests in *real* measurements, and (b) that the energy resolution predicted by our simulations is in fact close to what is experimentally observed.

We finally note, that over the last decade many new electro-optical devices have appeared that utilize multiple electrodes whose potentials cannot be readily obtained in analytical form. Examples include the segmented radial mirror analyzer [21] for scanning electron microscopy, the cylindrical mirror [22] and modified cylindrical mirror analyzers [23], the hyperbolic field analyzer [24] and others. Our electrode voltage optimization approach can be applicable in some form to these devices and therefore of a more general interest.

2. The biased paracentric HDA

The HDA is one of the most widely used electrostatic energy selectors (see Ref. [7] and references therein) as it can combine high energy resolution with good counting rates [7,12,17]. However, the first order focusing properties of the HDA at the dispersion axis are impaired by the fringing fields created at the HDA entry and exit electrode boundaries, leading to a substantial deterioration of its energy resolution [26]. Over the last decade, it has been shown in simulation, that this drawback can be readily overcome by using an arrangement that has come to be known as the *biased paracentric* HDA [16,26–29]. This type of HDA uses a biased optical axis (i.e. the central ray trajectory is not at zero potential) and an optimized entry position R_0 *offset* from the center position (at the mean radius $\bar{R} = (R_1 + R_2)/2$) utilized in conventional HDAs [7,17]. Thus, a biased paracentric HDA is nothing more than a conventional HDA whose entry has been displaced to either larger or smaller entry radius R_0 and whose electrode voltages have also been optimized by appropriately biasing its entry. The biggest advantage of this arrangement is that no additional fringing field corrector electrodes are needed. With the use of simulations [26,27,29] the optimal working parameters for the values of R_0 and bias voltage V_0 have been found. These simulations also showed that the expected energy resolution can be much improved. In a recent work these predictions were also tested experimentally on an HDA with entry and exit apertures (with lens and *real* entry aperture, but no PSD), specifically designed to this purpose [15]. The measurements showed a clear improvement of the experimentally-determined resolution for both negative and positive bias, in relatively good agreement with numerical results.