Journal of Electron Spectroscopy and Related Phenomena 177 (2010) 42–51

Contents lists available at ScienceDirect

Journal of Electron Spectroscopy and Related Phenomena

journal homepage: www.elsevier.com/locate/elspec

Fringing field optimization of hemispherical deflector analyzers using BEM and FDM

Omer Sise[a,*], Melike Ulu[a], Mevlut Dogan[a], Genoveva Martinez[b], Theo J.M. Zouros[c,d]

[a] Department of Physics, Science and Arts Faculty, Afyon Kocatepe University, 03200 Afyonkarahisar, Turkey
[b] Department Fisica Aplicada III, Fac. de Fisica, UCM 28040-Madrid, Spain
[c] Department of Physics, University of Crete, P.O. Box 2208, 71003 Heraklion, Crete, Greece
[d] TANDEM Accelerator Laboratory, Institute of Nuclear Physics, NCSR "Demokritos", 153.10 Aghia Paraskevi, Athens, Greece

ARTICLE INFO

Article history:
Received 1 December 2009
Received in revised form 20 January 2010
Accepted 25 January 2010
Available online 2 February 2010

PACS:
41.85.Qg
41.85.Ja

Keywords:
Hemispherical deflector analyzers
Fringing fields
Paracentric entry
Energy resolution
First-order focusing
BEM
FDM
SIMION

ABSTRACT

In this paper we present numerical modeling results for fringing field optimization of hemispherical deflector analyzers (HDAs), simulated using boundary-element and finite-difference numerical methods. Optimization of the fringing field aberrations of HDAs is performed by using a biased optical axis and an optimized entry position *offset* (paracentric) from the center position used in conventional HDAs. The described optimization achieves first-order focusing thus also further improving the energy resolution of HDAs.

1. Introduction

The trajectory of a charged particle moving in the field of an electrostatic energy analyzer is a subject of long-standing interest to experimentalists [1]. There continues to be a number of diverse fields where this problem is of paramount importance, as for example in the design of high-resolution electron spectrometers [2,3], space craft instruments [4], time-of-flight mass spectrometers [5], and electron microscopes [6] to mention only a few examples.

Hemispherical deflector analyzers (HDAs) combined with a cylindrical input-lens-system are widely used to analyze the energy of charged particle beams in collision physics [7–11], and are characterized by good energy and angular resolutions. In particular, the elimination of aberrations caused by the inherent fringing fields at the boundaries of electrodes is of primary concern. Fringing fields introduce departures from ideal field behavior leading to distorted trajectories, the degradation of first-order focusing and a corresponding loss in transmission. This is one of the main disadvantages of this type of analyzer. Over the past fifty years, traditional approaches to cure this problem have primarily sought to suppress these fields by improving field termination conditions typically requiring the unwieldy use of additional electrodes. The commonly used fringing field correctors such as Herzog [12], Jost [13], equipotential rings [14], and tilted input lens [15] mounted at the entrance and exit of the hemispheres reduce the effect of the electrostatic fringing field, but do not solve the problem, especially for spheres with a large interelectrode distance (≥50 mm). Analyzers using these correction methods have complex-shaped electrodes.

In 2000, Benis and Zouros [16] first showed that a simple displacement of the HDA entry from its conventional center position ($\bar{R}$) at ground potential to a new position $R_0 < \bar{R}$ with a positive entry bias ($V_0 > 0$) results in the restoration of first-order focusing without using any additional fringing field correctors. This is the result of the effective utilization of the intrinsic lensing proper-

* Corresponding author.
E-mail address: omersise@aku.edu.tr (O. Sise).

0368-2048/$ – see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.elspec.2010.01.003

ties of the fringing fields. This arrangement has been referred to as *positively* "biased paracentric entry" HDA (BPHDA). In Ref. [17], we extended their analysis and showed that there also exists a *negatively* BPHDA with $R_0 > \bar{R}$ and $V_0 < 0$. Very recently, we have reported on a detailed comparison of the commonly used fringing field correction schemes and showed that the biased paracentric entry configurations showed good focusing characteristics [18]. In this work, we give a physical interpretation of the lensing effect of the fringing field and propose a method for the numerical evaluation of the first- and second-order aberration arising in the fringing field regions of HDAs. Calculations of fringing field potentials are based on the boundary-element method (BEM) and the finite-difference method (FDM).

The work is organized as follows: In Sections 2.1 and 2.2, we introduce the HDA and present the analytical and numerical solutions for the ideal field. We compare the accuracy of simulated non-relativistic electron trajectories using BEM and FDM, and show that BEM results are extremely precise. Section 2.3 is devoted to the determination (numerically) of the fringing fields using BEM. In Section 3, we explain how ideal field trajectories are modified for fringing field cases, and show the efficacy of the new controlled lensing approach used in BPHDAs.

2. Hemispherical deflector analyzer

2.1. Ideal fields: analytical solution

Fig. 1 shows a cross section of an ideal HDA, where the deflecting electrostatic field is formed by the two concentric spherical surfaces of radii R_1 and R_2 at potentials V_1 and V_2, where 1 and 2 refer to the inner and outer spheres, respectively [19]. In the absence of fringing field effects, the electrostatic potential in the space between the two spheres, obtained from the solution of Laplace's equation, is given by

$$V(r,\theta,\varphi) = V(r) = -\frac{k}{r} + c, \tag{1}$$

where

$$\begin{aligned} c &= \frac{V_2R_2 - V_1R_1}{\Delta R} \\ k &= \frac{\Delta V}{\Delta R} R_1 R_2 \end{aligned}, \tag{2}$$

in which $\Delta R = R_2 - R_1$ and $\Delta V = V_2 - V_1$.

In an ideal field, the electron-optical properties can be derived from the trajectory of an electron subject to $V(r)$. Since the electric field and therefore, the force on the particle is proportional to $1/r^2$, the trajectory is a Kepler orbit [11,20].

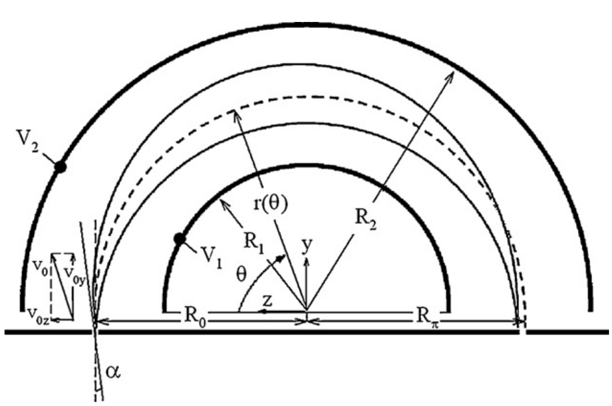

Fig. 1. Schematic cross section of a hemispherical deflector analyzer showing the various symbols used in the text.

For a particle emitted from the entrance of the HDA (r_0, $\theta_0 = 0$) with energy E and launching angle α, the solution of the particle trajectory inside the HDA, $r(\theta)$, is [11]

$$r(\theta) = r_0 \left[\frac{qk(1-\cos\theta)}{2r_0\cos^2\alpha\left(E - qc + \frac{qk}{r_0}\right)} + \cos\theta - \tan\alpha\sin\theta \right]^{-1} \tag{3}$$

and the exit radius r_π at $\theta = \pi$ is [11]

$$r_\pi = r_0 \left[\frac{r_0(E-qc)+qk}{qk\tan^2\alpha - r_0(E-qc)} \right]. \tag{4}$$

The voltage equations with respect to ground are obtained from [11]:

$$qV_i = E_0 \left\{ 1 - \frac{\gamma}{\xi} \left[\frac{R_0(1+\xi)}{R_i} - 1 \right] \right\} \quad (i = 1, 2), \tag{5}$$

where ξ is the HDA paracentricity defined as $\xi = R_\pi/R_0$, while γ is the bias (biasing parameter) defined as $\gamma = 1 - qV(R_0)/E_0$. Thus, a conventional HDA has $\xi = 1$ and $\gamma = 1$, while a BPHDA will have both $\xi \neq 1$ and $\gamma \neq 1$. Eq. (5) uniquely determines V_1 and V_2 in terms of potential $V(r_0)$ (or γ), the pass energy E_0 and the positions of the entrance R_0 and the exit R_π (or ξ), respectively. This is the most general formula for the voltages from which all specific cases may be derived.

The pass energy E_0 directly depends on the potential difference ΔV applied between the hemispheres causing the dispersing field, through [11]

$$E_0 = Cq\Delta V \tag{6}$$

$$C = \frac{R_1R_2}{\frac{\gamma}{\xi}(1+\xi)R_0\Delta R} \tag{7}$$

where C is the calibration constant [21].

Fig. 2 is a plot of the trajectories for ideal fields, as predicted by Eq. (3). This is the general equation of the particle trajectory within the ideal field HDA. Using Eq. (5), the potential was calculated for a configuration in which $R_1 = 75$ mm, $R_2 = 125$ mm, and $R_\pi = 100$ mm with R_0 taken as either centric 100 mm or paracentric 85 mm and 115 mm, respectively. These entry positions and HDA geometry were chosen to correspond to that of a spectrometer under construction in our laboratory with the particular entry positions determined in previous work [18] as having optimal focusing properties. Each trajectory group on the left side is made up of electrons which leave a point source at an angle α between $-5°$ and $5°$ (left) or between $-2°$ and $2°$ (right). The central group of orbits (right) has an energy ratio of $E/E_0 = 1$, while the upper orbits have 1.05 and the lower 0.95, respectively. The biasing parameter γ was taken to be 1.0 (i.e. unbiased) for the ideal field calculations. In the case of the ideal paracentric HDA biasing does not seem to have any distinct practical advantages over the conventional unbiased centric HDA [22].

An expression for the base width and base energy resolution of an HDA can be deduced from the differential equations of the trajectories in the deflector field. This can be obtained from the total differential relation of r_π [11]. The voltages on the hemispheres 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. 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 $r_\pi = R_\pi \pm \Delta r_\pi/2$ (notice that the base energy width ΔE is different from the FWHM resolution $\Delta E_{1/2}$ used elsewhere). Since $\Delta r_0/R_0$, $\Delta E/E$, and α^2 are all $\ll 1$, the exit beam width Δr_π is given