A parallel magnetic sector mass analyzer design

K.H. Cheong *, A. Khursheed

Department of Electrical and Computer Engineering, National University of Singapore, 4 Engineering Drive 3, 117576 Singapore, Singapore

1. Introduction

Khursheed et al. [1] presented a parallel magnetic sector analyzer design for electron energy spectroscopy. In this paper, the same kind of analyzer design is developed for mass spectroscopy applications. Khursheed et al. first presented simulated ray paths through an analytically generated field distribution, and then went on to find a viable parallel magnetic sector box analyzer design using 3D finite-element field solving programs. The same approach will be used here; only in this case, both energy and mass dispersion will need to be taken into account. A double-focusing electric sector/magnetic box analyzer will be presented. Also, due to the fact that ions have much larger masses than electrons, larger analyzer dimensions and deflection field strengths are used (than for the energy analyzer). Programs that take into account the effect of magnetic saturation are used to confirm the validity of simulation predictions based upon a simple magnetic scalar potential approach. As a general rule, the analyzer dimensions in the following work are scaled so that the maximum simulated deflection field strength lies below 1 T.

2. An analytically generated deflection field distribution

Following the Khursheed et al. [1] parallel magnetic energy analyzer design, trajectory paths of ions are first plotted through an analytically generated asymmetric Gaussian magnetic deflection field distribution, \( B_{\text{def}}(x,y) \), given by

\[
B_{\text{def}}(x,y) = B_0 \exp \left[ -\frac{(x-x_0)^2}{\sigma_x(x)} - \frac{(y-y_0)^2}{\sigma_y(y)} \right]
\]

where \( x_0 \) and \( y_0 \) are the x and y coordinates that define the position of maximum field strength, \( B_0 \); and \( \sigma_x(x) \) and \( \sigma_y(y) \) are standard deviations that describe how the function falls on either side of it in the x and y directions, respectively. Ions are deflected in the x–y plane, and the magnetic deflection field is applied in the z direction.

This paper presents a parallel magnetic sector mass analyzer design in which ions are simultaneously detected on a flat horizontal plane for a mass range of 1–260 amu. Simulation results predict that second-order focusing can be achieved for several regions in the detected mass spectrum. The analyzer is predicted to have an average mass resolution limited by spherical aberration of 611 for an input angular spread of \( \pm 25 \) mrad along its intrinsic focal plane, which when projected on a horizontal detector plane, drops to 371. For energy dispersion correction via the use of an electric sector, the average predicted mass resolution limited by spherical aberration (\( \pm 25 \) mrad angular spread) on the horizontal detector plane is 415. The predicted mass resolution limited by chromatic aberration is 592 where the energy spread is \( \pm 60 \) eV around an emission energy of 2 keV (\( \pm 3\% \)). A model based upon the magnetic scalar potential model is first used, and later checked by simulation that takes into account the effects of magnetic saturation.

© 2010 Elsevier B.V. All rights reserved.
1–260 amu were used. The mass resolution along the output focal plane is, as expected, higher than the predicted one for the straight-line detection plane. The analyzer is predicted to have an average mass resolution limited by spherical aberration of 205 for an input angular spread of $\pm 7.25$ mrad along its output focal plane, which when projected on to the horizontal detection plane, drops to 100. The curves in Fig. 3 reach a maximum value between 100 and 130 amu. Examination of the simulated trace-width distribution around this mass range (not given here) reveals the presence of second-order focusing. Elsewhere in the mass spectrum, the analyzer is characterized by first-order focusing.

3. A parallel magnetic box analyzer design

Following the parallel energy magnetic sector box design presented by Khursheed et al. [1], several different design layouts were investigated for mass spectrometer applications. The design most suited for parallel mass detection was found to be the second-order focusing magnetic sector box one reported by Khursheed [2], whose simulated deflection field distribution is shown in Fig. 4. Direct ray tracing of ion trajectory paths through this field distribution having 5, 10, 20, 50, 100, 150, 200 and 250 amu for an input angular spread of $\pm 25$ mrad and energy of 2 keV are shown in Fig. 5. A 3D magnetic scalar potential formulation is used here, where magnetic saturation effects are neglected. The ray
tracing techniques and finite-element programs used to generate these simulation results were written by Khursheed and are described in detail elsewhere [3]. The mass range varies from 1 to 260, and the size of the analyzer box is scaled up so that the maximum deflection field strength lies below 1 T. The detection plane in this mass analyzer design is different to the one for the second-order focusing energy analyzer reported by Khursheed [2], since the variation of masses along it, 1–260 amu, is considerably larger than the variation of energies along the output plane of the energy analyzer, 50–2500 eV. Fig. 6 shows the simulated mass resolution of the parallel magnetic box mass analyzer design. Like its corresponding energy analyzer design, it has several peaks, indicating that second-order focusing is predicted for many parts of the output spectrum.

It is important to investigate the focusing properties of the present magnetic box analyzer design in combination with some form of energy dispersion compensation. The conventional method, of using the energy dispersion of an electric sector to cancel the energy dispersion of a magnetic sector analyzer, only usually applies to a relatively small output mass range. In this case, cancellation of energy spread must take place across a wide output mass range, one that vary by three orders of magnitude. Ideal energy spread compensation characteristics for the magnetic box analyzer design can be found by plotting rays having different energies at different input heights, and noting their subsequent positions on the detector plane. A ray entering the box slightly higher than the central ray, will tend to focus a little distance before it on the detection plane, whereas a ray entering the box a little lower than the central ray, will tend to focus a little distance beyond it on the detection plane. Therefore, if there is an energy spread on the incoming ions into the box, they can be made to focus on to the same point on the detection plane (to a first-order approximation) if higher energy electrons enter the analyzer above the central ray, and lower energy electrons enter it below the central ray. The required dispersion in the entrance height, \( \Delta y \), is a function of input energy, \( \Delta E \), and by tracing rays at different heights and energies, ideal energy dispersion cancellation characteristics can be found for the magnetic box analyzer design. Simulation results show that a 1% variation in energy should be compensated by a corresponding 0.855 mm change in height, and that the change in height should vary approximately linearly with energy spread. Having established this, a suitable electric sector deflector can be designed, one which is predicted to provide precisely this energy dispersion on its output focal plane. Fig. 7 shows direct ray tracing of ions for such an electric sector together with the magnetic box analyzer design. On its output focal plane, the dispersion of the electric sector can be represented by the following energy and angular dispersion terms

\[
\Delta y = \frac{\Delta E}{E} C_C - C_i x^2
\]

where \( C_C \) is a chromatic aberration term and \( C_i \) is a second-order spherical aberration term. For the electric sector shown in Fig. 7, \( C_C = 85.5 \text{ mm} \) and \( C_i = 122.55 \text{ mm} \). The dimensions of the electric sector, \( R_1 = 6.8 \text{ cm} \) and \( R_2 = 10.25 \text{ cm} \) were scaled to provide the required energy dispersion. The source is placed close to the electric sector entrance in order to have near vertical focal plane at its exit. In addition a lens element is placed at the electric sector exit, in order to control the position of the focal plane in the horizontal direction, providing greater flexibility in creating the required dispersion condition. The internal deflector plate, \( V_D \), is 0.597 of the pass voltage (2 kV), and the middle electrode on the lens, \( V_L \), is set to be 1.2 times the pass voltage.

Fig. 8 depicts simulated ray paths around the detector plane for a monochromatic input beam, and a beam having a ±3% energy spread, with and without energy spread compensation. The mass range here is restricted to be between 5 and 50 amu for reasons of clarity, similar results are obtained for masses between 50 and 260 amu. These simulation results indicate that significant energy spread compensation is predicted for the magnetic box analyzer design. Fig. 9 quantifies this effect for the entire output mass range. It shows that the simulated mass resolution limited by an energy

---

**Fig. 5.** Simulated trajectory paths for ions having 5, 10, 20, 50, 100, 150, 200 and 250 amu through the magnetic box scalar potential design for an input angular spread of ±25 mrad. The source emission energy is 2 keV.

**Fig. 6.** Simulated mass resolution for the magnetic box scalar potential design for an input angular spread of ±25 mrad. The source emission energy is 2 keV.

**Fig. 7.** Simulated ion ray paths in a double focusing layout to minimize the effects of energy dispersion. The source ions are emitted at an energy of 2 keV, have a ±60 eV spread, and an angular spread of ±25 mrad. (a) Electric sector and parallel magnetic box analyzer and (b) electric sector alone.
The predicted mass resolution limited by 3% energy dispersion with compensation is 592, and is 33 without compensation. The average predicted mass resolution limited by spherical aberration (±25 mrad angular spread) on the horizontal detector plane is 415, better than the flat detector plane monochromatic case shown in Fig. 6, which has an average of 371, indicating that there is some degree of spherical aberration cancellation also taking place. The simulated trace-width as a function of input angular spread for selected masses is shown in Fig. 10. The trace-widths corresponding to peaks in the angular spread curve in Fig. 9, at masses 8, 100 and 230 amu, indicate the presence of second-order focusing (third-order spherical aberration variations), while at a mass close to its minimum value, say at 32 amu, there is first-order focusing (second-order spherical aberration variations).

A more realistic model of the magnetic box analyzer design was carried out by using the simulation program Lorentz 3EM [4], which can solve for magnetic field distributions in three dimensions, taking into account magnetic saturation effects. The 3D simulation model used in this case is shown in Fig. 11. Fig. 11(a) indicates the presence of Neodymium permanent magnets (darker regions) of differing heights in the z-direction, only half the box is shown. The coercive force ($H_c$) for these magnets is set to 11,250 AT/cm, and their $B$–$H$ curve characteristic as specified in the Lorentz 3EM program is shown in Fig. 11(b). The $B$–$H$ curve of all iron regions is also taken into account.

The height of each permanent magnet is adjusted to provide the same excitation strength set in the previous magnetic scalar potential design, shown in Fig. 4. Initial results indicated that the maximum field strength obtained by the inclusion of magnetic saturation is around 23% lower than the one obtained with the scalar potential model. To compensate this, the height of the strongest pair of magnets

---

**Fig. 8.** Simulated ray paths around the detector plane for the magnetic box scalar potential design for an input angular spread of ±25 mrad. (a) For a 2 keV monochromatic beam, (b) 120 eV (±60 eV) energy spread with no compensation and (c) 120 eV (±60 eV) electric sector energy spread compensation at analyzer entrance.

**Fig. 9.** Simulated mass resolution for the magnetic box scalar potential design for an angular spread ±25 mrad with and without energy spread compensation.

**Fig. 10.** Simulated trace-width distribution in the magnetic box scalar potential design for selected ions.

**Fig. 11.** 3D simulation model for the 3D magnetic field solving Lorentz program that takes into account permanent magnet $B$–$H$ curve (a) magnetic sector box analyzer (only half of box shown in the z-direction) and (b) $B$–$H$ curve specified for the permanent magnets.
is increased, changing its excitation strength from 14,400 to 20,000 AT, as shown in Fig. 12. The contours from this field distribution closely resemble those obtained from the previous scalar potential solution, and demonstrate that simple compensation for the effect of magnetic saturation can be made.

The effects of magnetic saturation become more difficult to circumvent when the dimensions of the magnetic box analyzer become smaller. Fig. 13 shows the simulated magnetic field distribution obtained by Lorentz 3EM for a 190-mm-long analyzer box design. Although the dimensions of the box are over a factor of 2.5 times smaller than the previous one, the maximum field strength still lies below 1 T. The dimensions and positions of the permanent magnets were changed, in order to obtain focusing on an approximately straight detector plane. The magnets are placed closer together in the x-direction, and an additional pair of magnets is inserted at the end of the box. Fig. 14 shows simulated rays paths of selected 1 keV ions through the smaller analyzer box design, indicating that the detector plane is now tilted. The focusing optics of the smaller analyzer box design is predicted to be considerably worse than for the 500-mm-long box. Fig. 15 shows simulated rays paths of 7, 8, 200 and 210 amu around the detector plane for an input angular spread of ±25 mrad. The calculated mass resolution from the 7/8 amu trajectories is 166, while for the 200/210 amu trajectories, it is 103. In general, the mass resolution varies between a minimum value of 62.5 to a maximum value of 200 for the mass range of 1–260 amu. The average predicted mass resolution limited by spherical aberration (±25 mrad angular spread) on the straight detector plane is 112. This value is over a factor of 3 times worse than the mass resolution of the 500-mm-long box design, which has an average mass resolution of 371 for the same mass range (see the flat focal plane curve in Fig. 6). While these preliminary simulations show that smaller parallel magnetic box analyzer designs (190 mm long) may be possible, the first indications from this investigation are that their focusing properties are likely to be worse than the bigger box analyzer designs (500 mm long).

4. Conclusions

This has presented parallel magnetic sector mass analyzer designs in which ions are simultaneously detected on a straight detector plane for a mass range of 1–260 amu. Simulation results predict that second-order focusing can be achieved for several regions in the detected mass spectrum. The analyzer is predicted to have an average mass resolution limited by spherical aberration of 611 for an input angular spread of ±25 mrad along its intrinsic
focal plane, which when projected on a horizontal detector plane, drops to 371. For energy dispersion correction via the use of an electric sector, the average predicted mass resolution limited by spherical aberration (±25 mrad angular spread) on the horizontal detector plane is 415. The predicted mass resolution limited by chromatic aberration is 592 where the energy spread is ±60 eV around an emission energy of 2 keV (±3%). A model based upon the magnetic scalar potential model is first used, and later checked by simulation that takes into account the effects of magnetic saturation. They predict that for a 500 mm long parallel magnetic box analyzer design, saturation effects can be compensated by readjustment of magnet excitation strengths. Preliminary simulation results indicate that although it may be possible to design smaller parallel magnetic box analyzers (190 mm long); their focusing properties are likely to be worse than the bigger parallel magnetic box analyzer designs (500 mm long).

References