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Reconstructing the Energy and Mass Spectra of Double-Focusing Spectrometers

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Abstract—We study the relation between the output signal and energy and mass distributions of charged particles at the input of tandem double-focusing mass spectrometers. A universal equation for arbitrary scanning methods is proposed. Formulas allowing the reconstruction of true energy and mass spectra are derived.

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INTRODUCTION

Tandem double-focusing mass spectrometers consisting of sequentially installed electrostatic and magnetic sector spectrometers (Fig. 1) are widely used to study the parameters of plasma and plasma–surface interaction. In these spectrometers, spectra are scanned by varying either the electrical or magnetic field (or both [1, 2], depending on whether the energy distribution or the isotopic composition of the particle flow is being measured).

Here we propose a universal equation for various regimes of spectrum scanning that links the signal at the output of the spectrometer with the energy and mass distribution of charged particles at its input. Based on this equation, we analyzed various algorithms of energy and mass spectra reconstruction.

MODEL

Our model is based on equations describing electrostatic and magnetic spectrometers, derived in [3, 4]:

$$I(U) = I_0 \int_0^\infty \delta(E) f(E) A_1\left(\frac{qU}{E}\right) dE,$$
$$I(H) = I_0 \int_0^\infty \delta(p) f(p) A_2\left(\frac{qH}{p}\right) dp, \quad (1)$$

where $f(E)$ and $f(p)$ are normalized particle distributions with respect to the energy and modulus of momentum at the input of spectrometer, respectively; $A_1\left(\frac{qU}{E}\right)$ and $A_2\left(\frac{qH}{p}\right)$ are the apparatus functions of electrostatic and magnetic spectrometers; $\delta(E)$ and $\delta(p)$ are the efficiencies of particle registration by the output detector; $I(U)$ and $I(H)$ are the signals at the output of the spectrometer; I_0 is the current at the input of the analyzer; q is the particle charge; H is the magnetic field strength in the magnetic spectrometer; and U is the electric potential on the electrostatic spectrometer plates. The particle energy to which the spectrometer is tuned and the particle momentum can be expressed in terms of the electric potential and magnetic field strength by relations

$$W = qk_1U, \quad p = qk_2H, \quad (2)$$

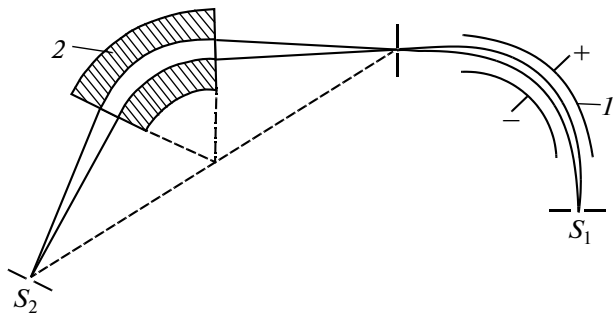
where k_1, k_2 are constants depending on the spectrometer's geometry.

Combining these equations for a tandem spectrometer, we have

$$I(U,H) = \sum_i I_{0i} \int_0^\infty \delta_i(E) f_i(E) A_1\left(\frac{q_iU}{E}\right) A_2\left(\frac{q_iH}{\sqrt{2m_iE}}\right) dE, \quad (3)$$

where summation is performed over all possible masses of particles.

To measure the energy spectrum of particles with fixed mass-to-charge ratio, one of the values is usually varied while the other one remains fixed. The spectrometer is then tuned to the maximum of one of the



Scheme of a tandem spectrometer: (*1*) electrostatic spectrometer, (*2*) magnetic sector spectrometer.

peaks, and the scanning regime is used to acquire the entire spectrum, in which

$$\frac{m_i U}{q_i H^2} = \text{const}. \quad (4)$$

The resulting signal is described by the equation

$$I(U) = I_{0i}\int_0^\infty \delta_i(E) f_i(E) A_1\left(\frac{q_i U}{E}\right) A_2\left(\sqrt{\frac{q_i U}{2E}}\right) dE = I_{0i}\int_0^\infty \delta_i(E) f_i(E) A\left(\frac{q_i U}{E}\right) dE. \quad (5)$$

The solution to Eq. (5) in the form of a series was obtained in [4]. In the first approximation, the solution is found by dividing the output signal by the scan voltage or, with allowance for (2), by the analyzer energy

$$f_i(q_i k_1 U) \approx \frac{B_0 I(U)}{q_i I_{0i} U \delta_i(q_i k_1 U)}, \quad (6)$$

where B_0 = const is a constant expressed in terms of the apparatus function moments. The relative energy resolution remains constant: $\Delta W/W$ = const.

The regimes of scanning with U = const or H = const are used to record mass spectra. In the standard procedure, peak intensities are measured at the flat top level, which imposes additional restrictions on spectrometer resolution. It was shown in [5, 6] that the isotope ratio can be effectively estimated from the peak area. However, these works considered a spectrum with a constant width and used a convolution equation valid for an exponential in a time scan, implying that we plot the mass spectrum on a logarithmic scale with respect to variables U and H. In the case of a linear scan with respect to voltage or magnetic field strength, this convolution equation is not applicable [4].

Equation (3) allows the reconstruction of a spectrum for this kind of scan. Additional normalization of the mass-to-change ratio is required for a signal processing algorithm based on simple calculation of the peak area, implying a priori knowledge of this ratio. There is, however, a reconstruction algorithm that does not require additional normalization with respect to mass.

For a fixed value of voltage applied to electrostatic spectrometer plates, scanning by varying magnetic field yields a series of peaks, each of which corresponds to a certain value of mass. Dividing equation (3) by H and integrating over the magnetic field under the assumption that the distribution function varies slowly within the width of the apparatus function of the electrostatic spectrometer, we obtain the approximate equation

$$\int_0^\infty \left(\frac{I_i(U,H)}{H}\right) dH \approx I_{0i} f_i(W)\delta_i(W) C_2 \int_0^\infty A_1\left(\frac{q_i U}{E}\right) dE \approx I_{0i} f_i(W)\delta_i(W) C_2 C_1 q_i U, \quad (7)$$

where W is the energy to which the electrostatic spectrometer is tuned: $W = q_i k_1 U$, C_1 and C_2 are constants.

Using Eq. (7) for peaks corresponding to different masses, it is easy to find relative content (weight) of these peaks for given energy. To find the relative content of a peak in this case, it is necessary to know a priori only the charges corresponding to the peaks, provided that the registration efficiency of various ions is the same:

$$\frac{I_{0n} f_n(W)}{I_{0i} f_i(W)} \approx \frac{q_i \delta_i(W) \int_0^\infty \left(\frac{I_n(U,H)}{H}\right) dH}{q_n \delta_n(W) \int_0^\infty \left(\frac{I_i(U,H)}{H}\right) dH}. \quad (8)$$

Let us consider an alternative method of reconstructing a mass spectrum for the same kind of scan, based on simple area calculation. Integrating equation (3) with respect to H yields

$$\int_0^\infty I_i(U,H) dH \approx I_{0i}\sqrt{2 m_i q_i} f_i(W)\delta_i(W) C_3 C_4 U^{3/2} \quad (9)$$

or

$$\frac{I_{0n} f_n(W)}{I_{0i} f_i(W)} \approx \frac{\delta_i(W) \int_0^\infty (I_n(U,H)) dH}{\delta_n(W) \int_0^\infty (I_i(U,H)) dH} \sqrt{\frac{m_i q_i}{m_n q_n}}. \quad (10)$$

Note that in contrast to Eq. (8), expression (10) contains mass in addition to charge, and each peak has to be identified with respect to charge and mass before the spectrum of an element can be reconstructed.

In addition to the above method of scanning the spectrum by varying the magnetic field, it is possible to fix magnetic field and scan the spectrum by varying the voltage applied to the electrostatic spectrometer plates. In this case, it is convenient to use an equation with integration over momentum instead of Eq. (3) with integration over energy:

$$I(U,H) = \sum_i I_{0i}\int_0^\infty \delta_i(p) f_i(p) A_1\left(\frac{2 m_i q_i U}{p^2}\right) A_2\left(\frac{q_i H}{p}\right) dp. \quad (11)$$

If the distribution function varies slowly within the width of the apparatus function of the magnetic spectrometer, we obtain the approximate equation

$$\int_0^\infty \left(\frac{I_i(U,H)}{U}\right) dU \approx I_{0i} C_5 C_6 f_i(p)\delta_i(p) q_i H, \quad (12)$$

or

$$\frac{I_{0n}f_n(p)}{I_{0i}f_i(p)} \approx \frac{q_i\delta_i(p)\int\limits_0^\infty\left(\frac{I_n(U,H)}{U}\right)dU}{q_n\delta_n(p)\int\limits_0^\infty\left(\frac{I_i(U,H)}{U}\right)dU}, \quad (13)$$

This equation allows us to find the relative content of peaks for a fixed value of momentum.

If the simple method of determining the peak area is used, we have

$$\int\limits_0^\infty I_i(U,H)\,dU \approx I_{0i}C_7C_8f_i(p)\delta_i(p)\frac{q_i^2H^3}{m_i} \quad (14)$$

or

$$\frac{I_{0n}f_n(p)}{I_{0i}f_i(p)} \approx \frac{q_i^2m_n\delta_i(p)\int\limits_0^\infty I_n(U,H)dU}{q_n^2m_i\delta_n(p)\int\limits_0^\infty I_i(U,H)dU}. \quad (15)$$

Each of expressions (9), (11), (13) and (15) allows us to determine the relative content of an element in the particle flow, but only expressions (9) and (13) do not require a priori knowledge of masses of elements.

CONCLUSIONS

Our results show that there is a simple method of energy spectrum reconstruction for different values of mass. This method, however, requires a priori knowledge of the element's charge. There are algorithms for determining the isotope composition of a flow of charged particles that require a priori knowledge of the charge of each element only, while our method based on simple calculation of the peak area requires knowledge of both the charge and the mass of each element.

Note that Eqs. (3) and (11) retain their form independent of the order in which spectrometers are combined in tandem, provided an electrostatic spectrometer without preliminary retardation is used. Hence, the spectrum reconstruction algorithms are equivalent in both cases. Eqs. (3) and (11) are applicable when an electrostatic spectrometer with preliminary retardation is used, provided the device is installed after the magnetic unit and is operated in the regime of a constant retardation factor in which the retardation potential and the potential applied to the deflecting plates are linearly coupled [3, 7].

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