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ESTIMATION OF THE BEAM WIDTH IN MAGNETIC MASS SPECTROMETER

O.N. Peregudov, E.A. Mironetz

Institute of Applied Physics NAS of Ukraine,
58, Petropavlivska Str., 40000 Sumy, Ukraine
E-mail: o.peregudov@gmail.com

A method for estimation of the beam width in magnetic sector mass spectrometers is proposed. This method consists in the restoration of the initial ion density distribution function in a beam cross-section before the receiving collector slit and can be used for the qualitative estimation of the mass spectrometer ion-optical scheme.

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1. INTRODUCTION

Precise measurements of the ion mass-to-charge ratio, as well as the ion abundance ratios, require careful adjustment of the mass spectrometer, the aim of which is to obtain the best focusing of the mass spectrometer ion-optical system. It is known [1] that one of the main parameters, using which the focusing quality is estimated, is the shape and size of the image of the ion source output aperture on detector. At the design stage of the ion-optical systems, parameters of this image are determined by the numerical simulation methods [2-5]. In the case of the operating device, to define the shape and size of the image one can use special mechanisms and equipment [6, 7].

In contrast to microprobe techniques, where image shape is determined by two-dimensional ion density distribution in a beam cross-section, in magnetic sector mass spectrometers during adjustment it is necessary to optimize the peak shape, which is the one-dimensional ion density distribution in a beam cross-section [2-4]. The perfect peak shape can be represented in the form of rectangle that corresponds to the passage of an infinitely narrow ion beam through the receiving collector slit. In real mass spectrometers perfect peak shape is inaccessible, since the ion density distribution in a beam reaching the collector is non-uniform and without sharp boundaries [1].

In the most of serially produced mass spectrometers it is impossible to determine the peak shape by the numerical simulation methods, since one cannot use a special equipment to determine the peak shape during adjustment of the mass spectrometer. Therefore, to estimate the width and non-uniformity of the ion density distribution function in the beam cross-section, operator should to calculate the resolution for different peak heights, to estimate the planeness of the peak top, and use other criteria as well. Directly operator makes a final decision concerning the acceptability of the peak shape.

The generalized model of the peak shape for magnetic sector and time-of-flight mass spectrometers, which allows to restore the ion density distribution in a beam cross-section before the receiving collector slit, is described in the work [8]. It gives the possibility to directly estimate the width and asymmetry of the ion density distribution function in a beam.

The present work is devoted to the application of the generalized model of the peak shape for the estimation of the beam width in a cross-section. We have shown that using a simple calibration procedure, it is possible to estimate the beam width in linear units.

2. EXPERIMENTAL PART

2.1 Mass spectrometer

Experiments were performed using mass spectrometer MI1201SG produced by "Selmi" (Sumy, Ukraine). Device is intended for the analysis of stable isotopes in gaseous phase with the sample ionization by an electron impact and is equipped by an ion receiver with two collectors (Faraday cups) – the main and additional ones. Additional collector corresponds to the ions with larger m/z ratio. There is the possibility in mass spectrometer to adjust the width of the ion source output slit and input slits of two collectors (or secondary-emission multiplier). Regulation is carried out using micrometer relocatable units, whose scale is not calibrated by the mass spectrometer producer. One knob turn has 50 points. The width adjustment range of the ion source output slit is from 0,05 mm to 0,5 mm, the collector slit widths are from 0 to 1,2 mm.

As a sample, we have used the standard krypton produced by "Ingaz" (Mariupol, Ukraine). Purity of the sample is 99,999%.

2.2 Determination of the peak shape parameters

From the mathematical point of view, the peak shape of a magnetic sector mass spectrometer can be represented in the form [8]

$$I\left(\tilde{m}\right) = \int\limits_{\tilde{m}\left(1-\rho^2-2\rho\right)}^{\tilde{m}\left(1+\rho^2+2\rho\right)} f\left(x-\mu\right)dx\,, \qquad (1)$$

where $\tilde{m} = m/z$ is the ion mass-to-charge ratio; $I\left(\tilde{m}\right)$ is the observed signal of the mass spectrometer; ρ is the dimensionless parameter characterizing relative increment of the ion turning radius, which corresponds to the half-width of a collector slit; μ is the peak position on the mass scale; $f(x)$ is the ion density distribution function in a beam cross-section before the collector slit. As an ion density distribution function, it is convenient to use the modified Gaussian function [9]

$$f\left(x\right) = \frac{A}{\sqrt{2\pi}\sigma}\exp\left(-\frac{k^2}{4} - \frac{\ln^2\left(1 + k\dfrac{x}{\sqrt{2}\sigma}\right)}{k^2}\right), \qquad (2)$$

where A is the peak area; k is the dimensionless parameter characterizing the degree of peak asymmetry.

Parameter σ in expression (2) can be used for the estimation of the peak width on the given height $h \in (0; 1)$

$$\Delta\tilde{w}_h = \begin{cases} \left|\dfrac{\sqrt{2}\sigma}{k}\left(\exp\left(k\sqrt{-\ln h}\right) - \exp\left(-k\sqrt{-\ln h}\right)\right)\right|, & k \neq 0, \\ 2\sqrt{2}\sigma\sqrt{-\ln h}, & k = 0, \end{cases} \quad (3)$$

where $\Delta\tilde{w}_h$ is the beam width (width of the ion density distribution function) expressed in the units of m/z.

It follows from the formula (1) that in the point $\tilde{m} = \mu$ the width of the collector receiving slit in the units of m/z is equal to

$$\Delta\tilde{w}_{sl} = 2\mu\rho\left(\rho + 2\right). \quad (4)$$

Using values $\Delta\tilde{w}_h$ and $\Delta\tilde{w}_{sl}$ it is possible to determine the coefficient of proportionality between the receiver slit width and width of the ion density distribution function in a beam on the given height

$$\alpha = \frac{\Delta\tilde{w}_h}{\Delta\tilde{w}_{sl}} = \frac{\Delta w_h}{\Delta w_{sl}}, \quad (5)$$

where values $\Delta\tilde{w}_h$ and $\Delta\tilde{w}_{sl}$ are expressed in linear units.

2.3 Estimation of the beam width by the peak shape simulation method

Estimation procedure of the beam width in a cross-section was the following. Peak of ^{84}Kr was registered for different positions of the adjustment knob of the collector slit width. At first, collector slit width increased by one complete turn of the knob till total slit opening. Thereafter the initial slit width was fixed. Then, slit width decreased sequentially by 10 points that corresponds to 1/5 of the turn. In the end of the experiment the initial slit width was restored. The chosen peak was scanned from the left to the right at each value of the slit width with minimum scanning step. The integration time was 0,1 s.

For each of the observed peaks the model parameters (1) were determined. Procedure was carried out by the standard Levenberg-Marquardt method, whose algorithm is realized in the GSL library [10]. We should to note that to provide a high efficiency of calculations, the library facilities need the assignment of analytical expressions for partial derivatives of the model.

Using the obtained parameters, for each peak we have defined the values of the beam profile full width at half maximum (FWHM) by the formula (3) and of the collector slit full width by the formula (4). Then the coefficient of proportionality was determined by the formula (5).

3. RESULTS AND DISCUSSION

In Fig. 1 we show the change in the relative increment of the ion turning radius ρ during the experiment.

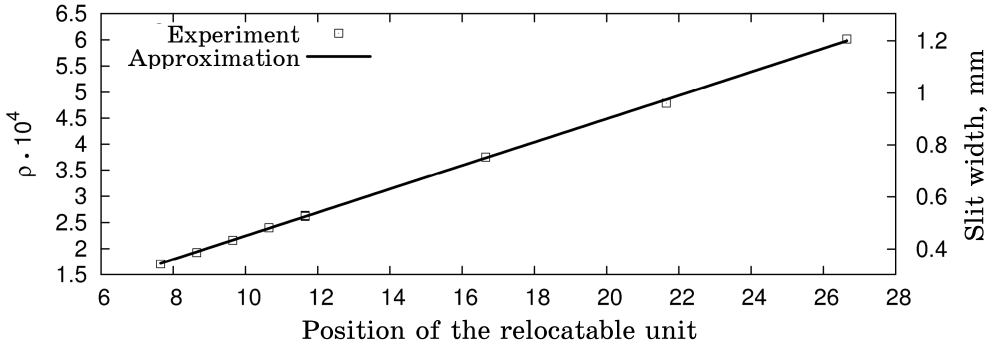

Fig. 1 *– Dependence of the parameter ρ on the position of relocatable unit knob of the collector slit width*

As seen from Fig. 1, the parameter value depends linearly on the position of the relocatable unit knob of the collector slit width. Taking into account this fact and the variation range of the slit linear sizes, which is specified in the device certificate, it is not difficult to realize the calibration for the collector slit width estimation in linear units over the stated spectrum. Result of such calibration is also represented in Fig. 1 (the scale is on the left).

Using the obtained dependence and the coefficient of proportionality, it is possible to estimate the beam profile FWHM in linear units for each peak. Results of the estimation are represented in Fig. 2.

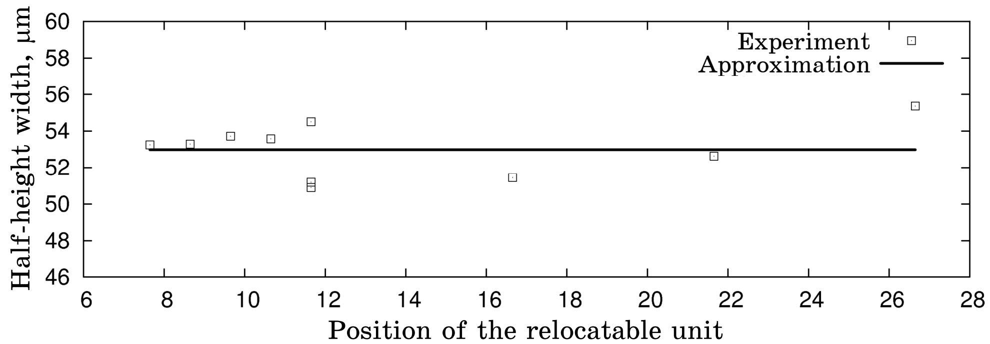

Fig. 2 *– Dependence of the beam profile FWHM on the position of relocatable unit knob of the collector slit width*

As seen from Fig. 2, the value of the beam profile FWHM does not depend on the position of relocatable unit knob and is about 53 μm. Indeed, conditions of the ion beam formation during experiment were not changed, and, therefore, the beam width should be approximately constant regardless of the collector slit width. It is also seen from Fig. 2 that the estimate spread is equal to some (of the order of 5) μm that can be explained by the relocatable unit play.

Determination of the beam width allows to choose correctly the detector slit sizes that is necessary for the provision of maximum transmission of an ion current from the ion source to the receiver [1]. Obviously, the detector slit width should be larger or equal than the beam width. However, during estimation of the beam width one should take into account the fact that the device producer does not calibrate the relocatable units of the collector slits. This will make the corresponding error to the obtained estimations, since deviations from the stated adjustment range are possible in a real device.

4. CONCLUSIONS

Application of the generalized peak shape model allows to sufficiently easily estimate the beam width on the given intensity level. In this case there is no need to use additional equipment. Moreover, the proposed technique substantially simplifies the mass spectrometer adjustment process, since it gives the possibility to estimate the focusing quality by two criteria: minimum width and minimal asymmetry of the ion density distribution function in a beam. Such simple criteria can be used while developing the automated computer systems of the mass spectrometer adjustment.

The proposed method can be successfully used for the development and upgrading of the magnetic mass spectrometer ion-optical schemes.

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REFERENCES

1. A.A. Sysoev, M.S. Chupahin, *Vvedenie v mass-spektrometriyu* (M.: Atomizdat: 1977).
2. L.N. Gall, V.D. Sachenko, *Int. J. Mass Spectrom. Ion Phys.* **46,** 43 (1983).
3. V.V. Laiko, A.F. Dodonov, *Rapid Commun. Mass Spectrom.* **8,** 720 (1994).
4. A.I. Boriskin, V.M. Eremenko, S.N. Mordyk, O.R. Savin, A.N. Skripchenko, V.E. Storizhko, S.N. Khomenko, *Tech. Phys.* **53,** 927 (2008).
5. H. Wollnik, *J. Mass Spectrom.* **34,** 991 (1999).
6. A.A. Ponomarev, V.I. Miroshnichenko, A.G. Ponomarev, *Nucl. Instrum. Meth. B* **267,** 2041 (2009).
7. S.E. Bragin, I.A. Vasilyev, O.M. Volodkevich, O.V. Grekhov, Yu.V. Kiselev, A.N. Mirzojan, V.A. Moiseev, A.V. Feschenko, *Problems of Atomic Science And Technology. Series: Nuclear Physics Investigations* No2(53), 96 (2010).
8. O.N. Peregudov, O.M. Buhay, *Int. J. Mass Spectrom.* **295,** 1 (2010).
9. R.D.B. Fraser, E. Suzuki, *Anal. Chem.* **41,** 37 (1969).
10. GSL-GNU Scientific Library, http://www.gnu.org/software/gsl/.