ION-OPTICAL CALCULATION OF TIME-OF-FLIGHT MASS-SPECTROMETER

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The parameters of shock mass-spectrometer for the dust particle composition analysis in near-Earth space are calculated. The time-of-flight mass-spectrometer of reflectron type is used as mass-spectrometer. The analytical expressions for particle trajectories in phase space in device different parts are obtained in paraxial beam approximation. The transmission value of device ion-optical system is calculated on the base of obtained expressions with the help of static modelling method. The device resolution is calculated and its dependence on mass-spectrometer parameters is defined.

Keywords: time-of-flight mass-spectrometer, cosmic dust, resolution.
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1. INTRODUCTION

The determination of cosmic dust chemical composition in near-Earth space by the analysis of shock plasma ion composition appearing at collision of the particle with solid (atom-pure) target [1] is the one of the methods of solid substance investigation.

The ion-optical parameters of mass-spectrometer used as the electrostatic time-of-flight mass-spectrometer (TFMS) are calculated in the given work. The choice of the given mass-spectrometer type is caused by the fact that it has some advantages in comparison with other schemes of mass-analyzers: the construction simplicity, wide range of investigated masses, high sensitivity, and high accuracy of quantitative analysis.

The electrostatic mirror which allows us to compensate the energy spread in ion beam is included into time-of-flight mass-spectrometer scheme for its resolution increase. Such device scheme is called mass-reflectron [2]. The electrostatic lenses which allow us to increase the device transmission though the device resolution decreases are included in the device scheme investigated by us [3]. But in some cases, the high transmission is the dominating condition of device scheme choice.

The variants of ion-optical schemes of the calculated device have the series of features of construction: grid count in ion source, target sizes on which the ionization of the investigated material takes place, the drift tube diameters and etc. Device consists of three main elements (fig.):

1. The ion source in which the primary formation of ions, their division in packets of different masses and introduction in analyzer take place. The source consists of target on which the investigated material ionization takes place and set of grids which are field-forming electrodes parallel to the target. In calculations the field between the grids is described as the field of plane capacitor.

2. The time-of-flight camera with electrostatic lens system in which the further division of ion packets and transformation of ion packet phase volume with the aim of device transmission increase. The electrostatic lenses are formed by tubular elements of time-of-flight camera between which the potential difference is formed. The lenses are thin ones for the given interval of potential variation on exciting electrode, i.e. their main plane coincides with the lens plane of symmetry.

3. The electrostatic plane mirror (reflector) formed by plane electrode system. The electrodes are made in the form of the grids in the joint of reflector with time-of-flight cameras. The series of auxiliary electrodes with linear potential distribution on them is put for the formation of more homogeneous potential distribution in reflector zone between main electrodes.

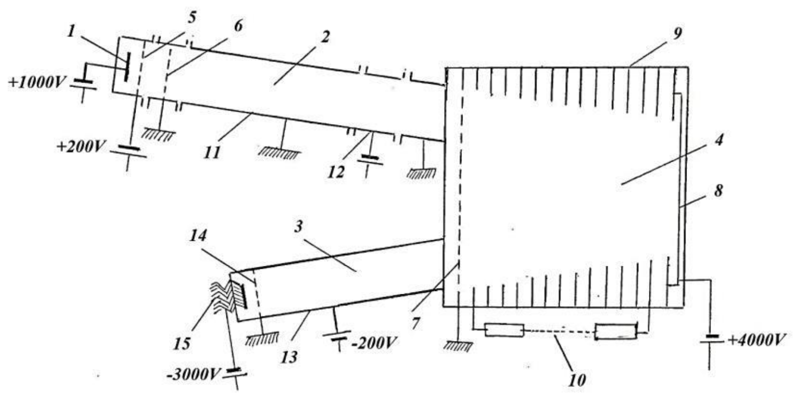

Fig. Mass-reflectron scheme 1 - is target; 2, 3 - are drift tubes, 4 - is reflector, 5 - is accelerating grid, 6 - is monitor grid, 7 - is reflector input grid, 8 - is reflector plane, 9 - is correction electrodes, 10 is voltage divider, 11-13 are focusing electrodes

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The accelerating gap for the energy increase of ions entering in detector is formed in the one of variants of calculated device scheme before ion detector, i.e., for increase of its sensitivity.

The values of the device resolution and transmission are the important parameters of mass-spectrometers. As the device dimensions have the final sizes then the part of the ions forming in the source are in its walls and are lost for the analysis. The quantity of such ions can consist of the significant part of forming ions. That's why the increase of device transmission values becomes the especially actual at few quantities of investigated material.

2. THE CALCULATION OF ELECTRO-FOCUSING SYSTEM TRANSMISSION VALUE.

The device transmission P value is defined as the ratio of ion number being in N_1 detector to ion number formed on N_0 target:

$$P = \frac{N_1}{N_0} \tag{1}$$

This ratio is calculated by static modelling method. It is supposed that the ion number in phase space element in ionization region has the form:

$$dN = const \cdot \exp[-V_{z0}^2 + V_z^2 + V_{\theta 0}^2] \cdot r_0 dr_0 dV_{z0} dV_{z0} dV_{\theta 0} \tag{2}$$

where $V_z, V_{z0,} V_{\theta 0}$ are the components of velocity vector in cylindrical coordinate system in the velocity space r_0 is the distance from the time-of-flight camera to the target, T is ion temperature.

Let's introduce the dimensionless values defined by the ratios for the convenience.

$$\rho = \frac{r}{R_d};\ v = \frac{V}{\sqrt{2\eta|W|}};\ r = t\frac{\sqrt{2\eta|W|}}{R_d};$$

$$\varepsilon_0 = \frac{E_0}{e|W|};\ W = -U_0;\ U_0 > 0$$

where R_d is the time-of-flight camera radius, v is ion velocities in drift field and ε_0 is the energy dimensionless value of the ions on the target; W is the potential difference between the source last grid and the target, U_0 is the target potential; E_0 is average ion energy on the target ($E_0 = 3/2kT$); $\eta = e/m$, e, m are the charge and mass of ion.

$$dN_0 = const \exp\left[-\frac{v_{r0}^2+v_z^2+v_{\theta 0}^2}{\frac{2}{3}\varepsilon_0}\right] \rho_0 d\rho_0 dV_{z0} dV_{r0} dV_{\theta 0} \tag{3}$$

moreover $v_{z0} \geq 0$, $\rho \leq \rho_m = R_0/R_d$, R_0 is the target radius.

The transformation of phase coordinates in ion source, drift gap in lens are defined by the following expressions:

a) in homogeneous field of ion source, the phase coordinates uniquely determine the state of a second-order system in terms of "k"

$$\rho_k^2 = (v_{r,k-1} \cdot \tau_k + \rho_{k-1})^2 + v_{\theta,k-1}\tau_k^2\ ,$$

$$v_{rk} = \frac{(v^2{}_{r,k-1} + v_{\theta,k-1}^2)\tau_k + \rho_{k-1} v_{r,k-1}}{\rho_k}, \tag{4}$$

$$v_{\theta,k} = \frac{\rho_{k-1}}{\rho_k} v_{\theta,k-1}\ ;\ \ v_{z,k} = \sqrt{v_{z,k-1}^2 + w_k}$$

where $\tau_k = 2\frac{d_k}{w_k}\left[\sqrt{v_{z,k-1}^2 + w_k} - v_{z,k-1}\right]$

$$w_k = \frac{U_k - U_{k-1}}{W};\ d_k = \frac{Z_k - Z_{k-1}}{R_d} \tag{5}$$

Z_k , U_k are coordinate and potential of k-th grid.
Z_0, U_0 are coordinate and potential of target.

b) in lens with power $P_j = -1/f_j$ (f_j is focal distance)

As the optical power of the lens for each ion is the same so we have

$$\rho_j = \rho_{j-1}$$

$$v_{r,j} = v_{r,j-1} + P_j \rho_{j-1} v_{z,j-1}\ ;$$

$$v_{\theta,j} = v_{\theta,j-1};\ v_{z,j} = v_{z,j-1} \tag{6}$$

The transformation of phase coordinates in reflector at transmission calculation is accepted as the equivalent to the one in drift gap by the length:

$$S_p = 4d_r \cdot \frac{U_0}{U_r}$$

where U_r the voltage on reflector is, d_r is reflector depth.

Thus, the transformation of phase coordinates in the considered device can be presented as consistent transformation of (2)–(4) type. This consistence is defined by device scheme.

The distribution type function (1) is modeled with the help of standard gauge of random numbers. After each transformation (2), (3) the condition of ion transmission through device element is checked and ions with $\rho \geq 1$ is excluded from the further consideration.

3. THE CALCULATION OF THE DEVICE RESOLUTION

The ratio of average run time τ_0 from the target up to the double value of time spread of fixed mass ion receipt on detector:

$$R = \frac{\tau_0}{2\Delta\tau} = \frac{m}{\Delta m}$$

The static modelling method allows us to calculate the device resolution but makes difficult the definition of the dependence of its value on device parameters. That's why in the given work R is obtained on the base of obtained analytical expressions.

The time of motion of the ion emitted with $\mathcal{E}_0$ initial energy under angle φ_0 to normal of output diaphragm in the source with one grid is equal:

$$\tau_U = 2d_1(\sqrt{1+\mathcal{E}_0 cos^2\varphi_0} - \sqrt{\mathcal{E}_0}cos\varphi_0) \quad (7)$$

with two grids is equal:

$$\tau_U = 2\frac{d_2}{w_2}\left(\sqrt{1+\mathcal{E}_0 cos^2\varphi_0} - 2\frac{d_1}{w_1}\sqrt{\mathcal{E}_0}cos\varphi_0\right) + \\ +2\left(\frac{d_1}{w_1} - \frac{d_2}{w_2}\right)\sqrt{w_1 + \mathcal{E}_0 cos^2\varphi_0} \quad (8)$$

The ion motion time in drift field gap by S_i length without lenses is [4]:

$$\tau_i = S_i - \frac{\mathcal{E}_0}{2}S_i \quad (9)$$

The motion time in the reflector is:

$$\tau_r = \frac{4U_0}{E \cdot R_d}\sqrt{1+\mathcal{E}_0}(sin\varphi_1 \cdot sin\beta \cdot cos\text{æ} + \\ +cos\varphi_1 \cdot cos\beta) \quad (10)$$

where E is absolute value of electric field strength in reflector; $\varphi_1$is the angle between ion velocity vector and Z tube axis at the output in reflector; æ is the angle at the output in reflector between ion velocity vector component perpendicular to Z axis and X axis being in the device meridional plane; β is the angle between Z and reflector axes.

The motion time in detector accelerating gap:

$$\tau_D = \frac{2d_D}{w_D}\left(\sqrt{1+\mathcal{E}_0+w_D} - \sqrt{1+\mathcal{E}_0}\right) \quad (11)$$

where $w_D = \frac{U_D}{W}$

Expanding the expressions (7), (8), (10), (11) into series over $\mathcal{E}_0$ and taking under consideration only 1st expansion order we obtain the following formula for each device element:

$$\tau = \tau_0 + \mathcal{E}_0 \cdot \tau_{\mathcal{E}} + \Delta\tau \quad (12)$$

where $\mathcal{E}_0 \cdot \tau_{\mathcal{E}}$ and $\Delta\tau$ are ion packet broadening by coordinate because of the spreads by energy and by angles correspondingly.

Then, we obtain the following expressions for (12) formula components for single-grid source for device different parts:

$$\tau_{0U} = 2d_r, \tau_{\mathcal{E}U} = d_1$$

and

$$\Delta\tau_U = 2d_1\sqrt{\mathcal{E}_0}(1 - cos\varphi_{0m})$$

where φ_{0m} is maximal angle between velocity vector ions and tube axis on target (for ions reached the detector) for the drift gap S_i , $\tau_{0i} = S_i$.

The reflector allows us to compensate the energy spread in ion packet. The focusing condition of first order by the energy in detector plane is defined from the condition:

$$\frac{\delta\tau}{\delta\mathcal{E}_0} = \tau_{\mathcal{E}} = \tau_{\mathcal{E},U} + \sum_i \tau_{\mathcal{E},i} + \sum_j \tau_{\mathcal{E},j} + \tau_{\mathcal{E},R} + \\ + \tau_{\mathcal{E},D} = 0 \quad (13)$$

then the device resolution is equal:

$$R = \frac{\tau_{0U} + \sum_i \tau_{0i} + \sum_j \tau_{0j} + \tau_{0R} + \tau_{0D}}{2(\Delta\tau_U + \Delta\tau_R)} \quad (14)$$

If we neglect the time-of-flight times in the source and detector, then from (14), (15) we obtain the following approximate formula:

$$R = \frac{1}{2\varphi_{1m}} \cdot \frac{cos\beta}{sin\beta} \quad (15)$$

Formula (15) gives the practically similar results (maximal difference 2,5 %) for the considered device parameters.

The calculation results for ion shock plasma having the energy of directed motion 1keV and heat motion 5eV are presented in table.

Table

The calculation results for ion shock plasma parameters having the energy of directed motion 1keV

Parameter	With lenses	Without lenses
P	9,1%	5,4%
R	2,61%	3,63%
U_R	1,17%	1,7%
$\Delta\tau_0$	66,82%	66,82%
$\Delta\tau$	0,128%	0,092%
φ_{0m}	0,32%	0,23%
φ_{1m}	0,22%	0,016%

The ion time of flight value can be found by the following formula:

$$t = R_d\sqrt{\frac{M}{Z \cdot U_0}}\tau \cdot 0{,}723 \cdot 10^{-6} \quad (16)$$

Here R_d is expressed in centimeters, M is expressed in proton masses, Z is expressed in electron charges, U_0 is expressed in volts. For example, from (16) it is followed that $Z = 1$ average time-of-flight t_0 is 40,1µs and time spread of ion receipt on detector is 77 *ns* at M =109.

4. CONCLUSION

Thus, the previous experiments show that characteristics of developed mass-reflectron correspond to problem methodical aspects and also to structural and technological device developmental work. The mass-reflectron parameters are given below:

Velocity range km/sec	3-35
Mass range, gr	10^{-14}-10^{-12}
Range of registered mass numbers, amu	12 – 75
Resolution (for Fe^{56}) at level 10%	not less 200
Sensitivity by Fe^{56} Kl/kg	not less 200

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