

Reconstructing Energy Spectra in Spectrometers with Preretardation using Diaphragms with Round Holes

V. A. Kurnaev* and V. A. Urusov

Moscow Engineering Physics Institute (State University), Moscow, 115409 Russia

*e-mail: kurnaev@plasma.mephi.ru

Received November 12, 2009

Abstract—A relationship between the energy distribution of particles and the analyzer output signal has been studied for energy-dispersive electrostatic spectrometers with a preretardation system consisting of diaphragms with round holes. The theoretical model is compared to the results of computer simulations and experimental data. A simple formula is proposed for reconstructing the true energy distribution at low values of the retarding ratio.

DOI: 10.1134/S1063785010050196

Most of the modern electrostatic spectrometers are equipped with a system of preretardation [1–3]. These spectrometers are usually employed in one of two regimes. In the first regime, called the constant retarding ratio (CRR) mode, there is a linear relationship between the analyzer energy and the retarding potential. In the second regime, called the constant analyzer transmission (CAT) mode, the analyzer energy is set constant and the spectral sweep is achieved by varying the retarding voltage. The operation of electrostatic spectrometers with preretardation was analyzed in monograph [1]. In addition, a number of investigations were devoted to studying the influence of various factors on the energy resolution and transmission function of these spectrometers by means of computer simulations [4–6]. However, no attempts of theoretical analysis of the relationship between the energy distribution of particles and the analyzer output signal have been reported until now, and no algorithms were proposed for reconstructing the true energy distribution.

Previously, it was shown [7] that, provided the mutual proportionality of potentials on the spectrometer electrodes, the current of charged particles $I(U)$ at the analyzer output and their energy distribution $f(E)$ at the input in the CRR mode are related as follows:

$$I(U) = \int_0^{\infty} A\left(\frac{qU}{E}\right) f(E) dE, \quad (1)$$

where $A(qU/E)$ is the transmission function of the analyzer. Assuming that the energy distribution only slightly changes within the width of the transmission function, we infer from Eq. (1) that the integral of this function is proportional to analyzer energy $W = kqU$, where q is the particle charge and k is the proportion-

ality coefficient that depends on the system geometry [7].

In a CAT mode, no such universal relationship exists. In some cases, the integral of the transmission function is inversely proportional to the analyzer energy [8], but it was repeatedly demonstrated in experiments [2, 3, 9–11] that this integral can be described approximately by the square root of the energy (see, e.g., a review in [3]).

The aim of this investigation was to analyze the influence of preretardation in electrostatic spectrometers on the relationship between the energy distribution of particles and the analyzer output signal in spectrometers with the transmission limited by geometric factors.

A simple model of a spectrometer with preretardation comprises a retarding system (two or three diaphragms with round holes) and a dispersive energy analyzer (Fig. 1). The angular distribution of particles at the entrance of the preretardation system will be considered approximately isotropic within an angular aperture viewed by the analyzer. Assuming that the energy distribution rather insignificantly changes within the width of the transmission function, we obtain the following approximate equation [7]:

$$I(U, U_1) \approx f(W) \int_0^{\infty} A\left(\frac{qU}{E}, \frac{q(U-U_1)}{E}, \frac{q(U+U_1)}{E}\right) dE, \quad (2)$$

where $W = qU + kqU_1$ is the analyzer energy set in the given case, U is the retarding potential, and U_1 is the potential on the analyzer electrodes relative to the retarding input diaphragm. Provided that the transmission function of the retarding system also weakly varies within the width of the transmission function of the analyzer and the angular distribution of particles at

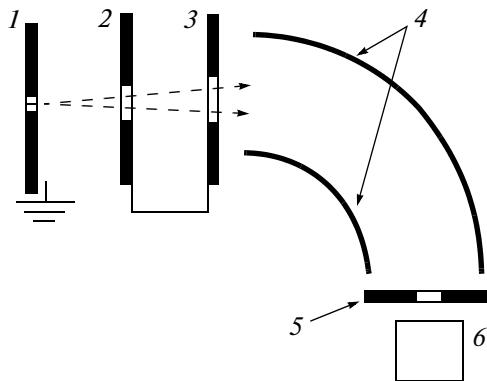


Fig. 1. Geometric model of an energy-dispersive electrostatic spectrometer with a preretardation system: (1) input diaphragm; (2) first collimating diaphragm; (3) second collimating diaphragm; (4) dispersive energy analyzer; (5) output diaphragm; (6) detector.

the entrance of the analyzer insignificantly influences the integral of the transmission function, Eq. (2) can be simplified to

$$\begin{aligned} I(U, U_1) &\approx f(W) \int_{qU}^{\infty} A_1\left(\frac{qU}{E}\right) A_2\left(\frac{-qU_1}{E-qU}, \frac{qU_1}{E-qU}\right) dE \\ &\approx f(W) A_1\left(\frac{qU}{W}\right) C q U_1, \end{aligned} \quad (3)$$

where

$$C = \int_0^{\infty} A_2(1/z) dz = \text{const},$$

and $A_1(qU/W)$ is the transmission function of the retarding system.

The transmission function of the retarding system strongly depends on the system geometry. Let us consider a simple model with a small input hole and the isotropic angular distribution of particles at the entrance. With neglect of the potential sagging in the hole, the transmission function of the retarding system can be determined as the ratio of the solid angles in which the particles are transmitted via diaphragms at a given retarding potential U and at $U = 0$. In a small-angle approximation, this transmission function is as follows:

$$A_1\left(\frac{qU}{W}\right) = \frac{\Omega}{\Omega_0} \approx \frac{(1 + \sqrt{1 - qU/W})^2}{4}, \quad (4)$$

where Ω_0 is a solid angle in which the particles are transmitted via collimating diaphragms at $U = 0$.

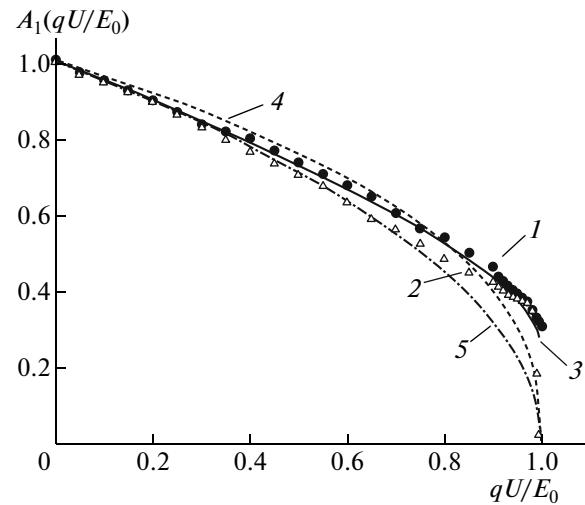


Fig. 2. Plots of the transmission function of the retarding system versus retarding potential: (1) Simion 3D profile after the first collimating diaphragm; (2) Simion 3D profile after the second collimating diaphragm; (3) Eq. (4) of the proposed theoretical model; (4) $(1 - qU/E_0)^{0.4}$ approximation of experimental data [3]; (5) $(1 - qU/E_0)^{0.5}$ approximation of experimental data [11].

Expression (4) is valid for the retarding potential in varied within the following limits:

$$0 < U < \frac{W/q}{1 + \tan^2 \theta_0/4}, \quad (5)$$

where θ_0 is the maximum angle at which the particles are transmitted via the retarding system. Outside this interval, the character of the transmission function of the retarding system changes. According to calculations, it must linearly decrease until vanishing. However, the transmission function is also significantly influenced by stray fields. For this reason, the character of the transmission function outside interval (5) may differ from linear decay.

The results of theoretical modeling were compared to the results of numerical simulations obtained using Simion 3D routine. As can be seen from Fig. 2, there is good qualitative and quantitative coincidence between these results for small hole diameters and, hence, small sagging of the potential. For greater holes, the potential sagging leads to a nonmonotonic variation in the region of large values of the retarding ratio (Fig. 3), which is related to the focusing effect of stray fields. In practice, the stray field effects are decreased by using grids, which allows formula (4) to be used at greater values of the retarding ratio.

One standard method of calibrating spectrometers is based on the use of a monoenergetic plane-parallel beam of particles. The results of numerical simulations using Simion 3D routine for such plane-parallel beam of particles at the input shows that the transmission

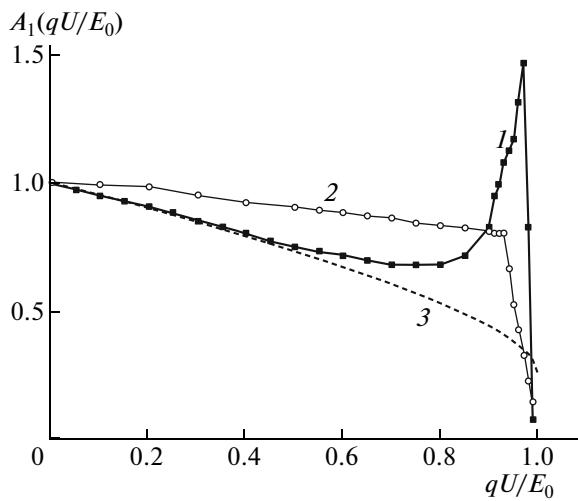


Fig. 3. Transmission function of the retarding system (1) numerically simulated for the model geometry with a hole in the second collimating diaphragm smaller than that in the first one, (2) numerically simulated for a monoenergetic plane-parallel beam of particles at the entrance of the retarding system, and (3) theoretically approximated using Eq. (4).

function of the retarding system weakly changes in a broad energy range. At large values of the retarding factor, this dependence becomes almost linear (Fig. 3). Therefore, the conventional experimental calibration of a spectrometer can lead to a transmission function that deviates from the true one, in particular, for investigations of the interaction of charged particles with a sample surface, in cases where the size of a probed region is greater than the size of a region viewed by the analyzer.

In conclusion, the results of this investigation lead to the conclusion that no universal relationship between the analyzer response signal (current) and the energy distribution of particles exists in the CAT mode (in contrast to the CRR mode). However, for a given spectrometer geometry (Fig. 1), the true energy spectrum in both CRR and CAT modes can be reconstructed using formulas (3) and (4).

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Translated by P. Pozdeev