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Ionization efficiency calculations for cavity thermoionization ion source

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Abstract

The numerical model of a thermoemission ion source was used for source ionization efficiency calculations. The dependency of ionization efficiency on working parameters like ionizer length and extraction voltage was discussed, and a good agreement with theoretical predictions was achieved. It was shown that increasing the ionizer length does not significantly change the obtained ionization efficiency. Extraction voltages up to a few thousand of volts are sufficient to obtain reasonable efficiency.

Keywords: Ion sources; Computer simulation; Electromagnetic isotope separation

1. Introduction

Thermoemission ion sources of various designs are widely used in electromagnetic isotope separation [1–4]. Their characteristic features are: high working temperature (2500–3300 K) and small dimensions of the ionization chamber, also known as the ionizer. Ion beams obtained from these sources are relatively pure due to the absence of multicharged and residual gas ions. However, the main advantage of thermoemission ion sources is their high ionization efficiency and the small amount of substances needed to obtain a stable ion current.

The main part of the source is the cylindrical, semi-opened ionizer of length L and radius r. It is made of a metal with high melting point (e.g. tungsten) and heated to the working temperature by electron beams from tungsten cathodes. Ions are extracted using an extraction electrode at the potential $-V_{ext}$. During on-line experiments, the ionizer is simultaneously an irradiated target, in which nuclear reactions induced by high-energy protons take place.

Atoms produced in nuclear reactions inside the ionizer wall diffuse to the ionizer's cavity. Colliding with walls of temperature T, they undergo surface ionization with an ionization degree α given by the Saha–Langmuir equation [5,6]. Another quantity, the ionization coefficient $\beta = \alpha/(1+\alpha)$ is defined as the probability that a particle undergoes ionization. It should be stressed that the above-defined quantities describe a single ionization act. They should not be mixed up with ion source ionization efficiency, understood as the ratio of the number of extracted ions N^{+*} to the number of the atoms introduced into the ionizer N_o:

$$\beta_w = N^{+*}/N_o.$$

In our previous paper [7], a simple theoretical model of thermoionization ion source work was described. The model was based on the assumption that an atom touching the hot ionizer surface is ionized with probability β and then desorbs, moving in the direction determined by the cosine angular distribution with respect to the normal. Initially, the extraction field was neglected. In that case, atoms and ions move with a constant velocity until they hit the ionizer wall or pass the extraction opening and $\beta_w = \beta$ occurs. Then the assumption was made that the extraction field inside the whole volume of ionizer was strong enough to remove every produced ion immediately after ionization. For such a working mode, the source ionization efficiency calculated in the frame of the discrete model may be much greater than β from the Saha–Langmuir formula.

The aim of this paper is to calculate the thermoionization ion source efficiency for more realistic working conditions, when the extraction field penetrates the ionizer

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volume at some finite depth, and consequently, not every ion is extracted immediately after its creation. These calculations are done by means of computer simulations. One may suppose that using an extraction voltage V_{ext} would result in the ionization efficiency exceeding β. The simulation results will be compared to the theoretical predictions. The simulations have been performed for various L (the radius was kept constant) in order to check the influence of ionizer's elongation on ionization efficiency. The changes of efficiency due to the changes of extraction voltage were also investigated.

2. The numerical model

The Monte Carlo method-based code follows trajectories of particles in the ionizer cavity. The flat extraction electrode is on the potential $-V_{ext}$ with respect to the ionizer. The electrostatic field from the electrode penetrates the ionizer volume and influences the trajectories of ions. A homogeneous field directed along the ionizer axis may be also set in the code. The simulation area is covered with a 3D Cartesian spatial grid. The dimensions of cells are $\Delta x = 0.2$ mm and $\Delta y = \Delta z = 0.1$ mm. The grid has 100 cells in the y and z directions; its size in the x direction depends on the ionizer length. The electrostatic potential is determined by solving the Laplace equation. This is done using the successive over-relaxation technique [8]. The electrostatic field strength values at the grid nodes are calculated by numerical differentiation of potential.

Particles are emitted from the internal surface of the ionizer chamber according to the cosine distribution of their velocity direction with respect to the normal. The values of initial velocities correspond to the temperature $T = 2500$ K. Neutral particles move with a constant velocity. Trajectories of ions are influenced by the electrostatic field. The equations of motion are solved using the fourth order Runge–Kutta method [9]. When the code detects that a particle hit the ionizer wall, the Monte-Carlo-based subroutine decides whether the particle is ionized/neutralized or not, according to the β parameter. The new initial velocity is determined and the particle continues its journey until it leaves the ionizer. The code counts the ions and neutral atoms leaving the ionizer and calculates the ionization efficiency.

3. Simulation results

Initially, test simulations of the ion source without an extraction field were performed. The simulations were done with an ensemble of 10^5 particles introduced into the ionizer. The dependency of the source ionization efficiency on the ionization coefficient β was investigated for an ionizer of length $L = 8$ cm and radius $r = 0.4$ cm. The value of β coefficient changed in the range 0.01–1. The lowest line in Fig. 1 represents the dependency obtained from simulations. It perfectly matches the theoretical $\beta_w = \beta$ dependence.

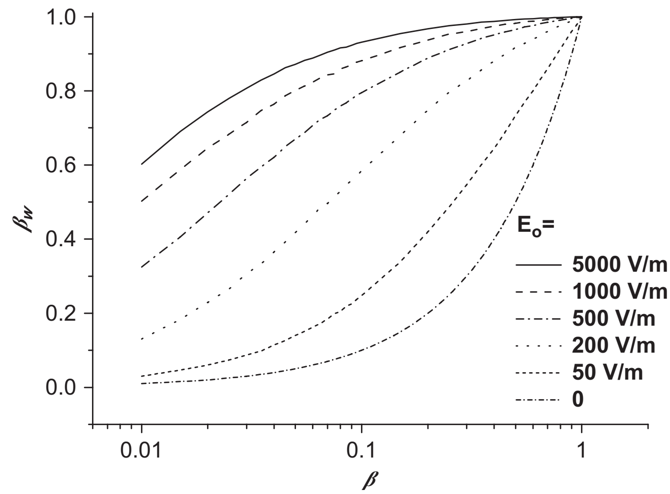

Fig. 1. Ionization efficiency as a function of β parameter in the case of homogeneous extraction field.

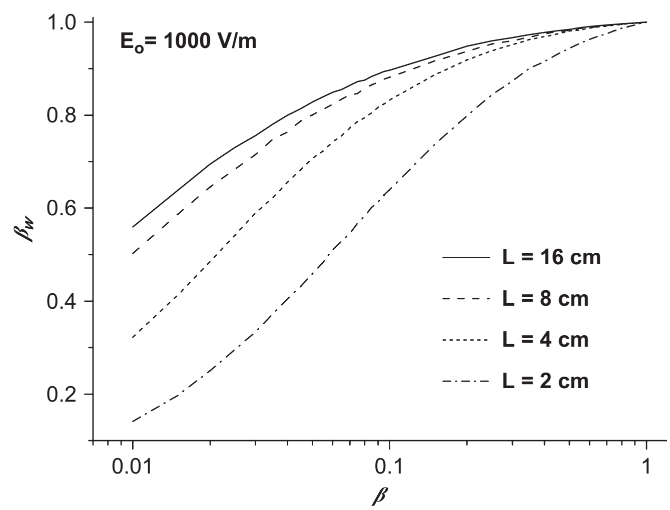

Fig. 2. Ionization efficiency as a function of β parameter for different values of ionizer length, for the case of homogeneous extraction field.

Next, a homogeneous extraction field directed along the ionizer axis (x-axis) was assumed. Calculations have been done for field strengths up to $E_o = 5$ kV/m, when the ionizer works very close to 'each-ion' regime. The results are presented in Fig. 1. It is easy to see that even a relatively weak field of $E_o = 50$ V/m causes a remarkable increase of source efficiency.

The change of ionization efficiency due to an increasing elongation of the ionizer was also investigated. Simulations were done for $E_o = 1$ kV/m and various L values. It can be seen (Fig. 2) that the smaller the β of the ionized substance, the larger the influence of L. It should be noted that for large values of β, effects due to the ionizer elongation are of minor importance.

After the analysis of the limiting modes of ionizer's work, the more realistic model of extraction field from the flat extraction electrode on $-V_{ext}$ potential is considered. The region penetrated by the extraction field is crucial for obtaining a larger ionization efficiency. Particles which are moving far from the opening do not feel the extraction field and roam inside the ionizer, changing direction of motion randomly during collisions with walls. On the other hand, when a charged particle reaches (or is created in) the extraction area, its movement is directed towards the extraction opening. In the extraction region close to the opening, the work of the ionizer is close to the 'each-ion' regime. Fig. 3 presents $\beta_w(\beta)$ dependencies for different values of V_{ext}. Even a very small value of $V_{ext} = 100\,\mathrm{V}$ gives quite a satisfactory increase of β_w compared to the 'no-field' case. One could expect that these further increases of V_{ext} would lead to dramatically larger efficiencies. But this is not true, as can be seen in Fig. 4 (25% increase of β_w when V_{ext} increases 100 times). Excessive increases of V_{ext} are pointless, especially taking into consideration technical difficulties.

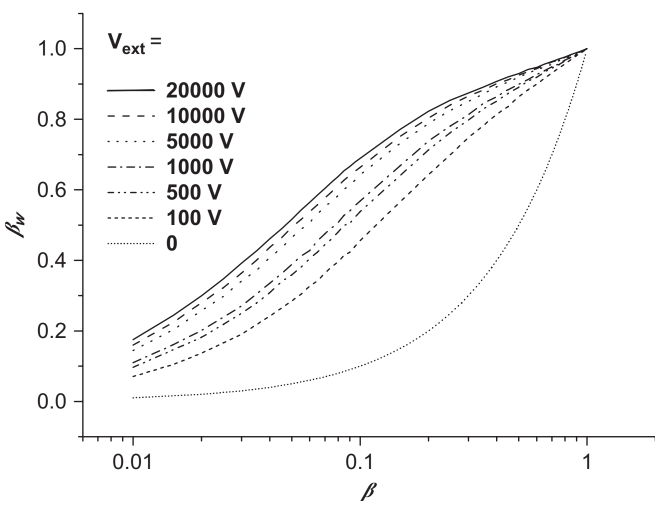

Fig. 3. Ionization efficiency as a function of β parameter in the case of realistic extraction field.

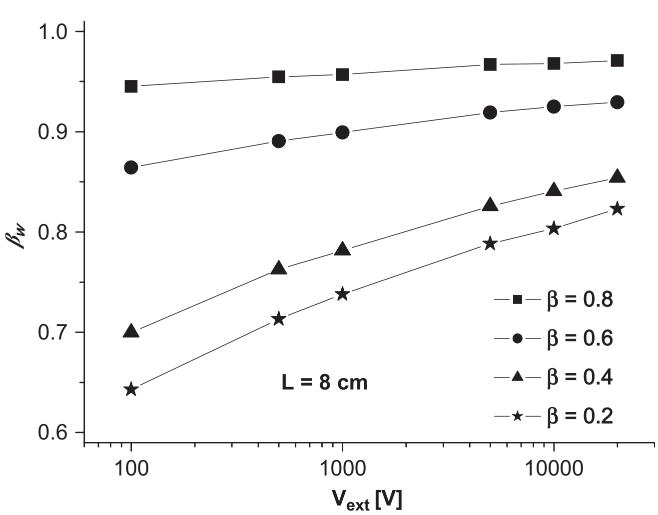

Fig. 4. Dependency of ionization efficiency on the extraction voltage V_{ext}, for the case of realistic extraction field.

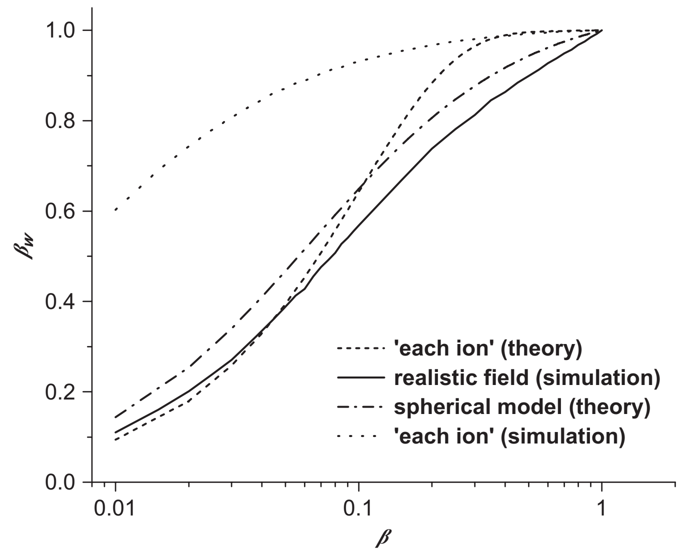

Fig. 5. Comparison of ionization efficiency $\beta_w(\beta)$ obtained from simulations and predicted by theoretical formulae.

In the case of realistic extraction field, large elongations of the ionizer are not desirable. One can observe a slight decrease of ionization efficiency when L grows. This can be understood when one bears in mind that the extraction field enters the ionizer at the depth of approximately 1 cm.

The simulation results are compared to the theoretical predictions in Fig. 5. The 'each-ion' formula from [7] describes very good $\beta_w(\beta)$ dependence for 'each-ion' simulations with the homogeneous $E_o = 5\,\mathrm{kV/m}$ field for $\beta > 0.3$. The simplifying assumption of the theoretical model that non-charged particles drift towards the extraction opening could be the reason for discrepancies for smaller β. The simulation results in the case of realistic field are similar to those predicted by the 'spherical-ionizer' formula [7]. The trends of both curves are almost the same. The discrepancies may be caused by the assumption of spherical ionizer shape.

4. Conclusions

The numerical model of thermoemission ion source described in the paper makes a possible much more realistic description than that presented in our previous paper [7]. The calculations of β_w for realistic extraction fields were performed. The results are in a good agreement with the 'spherical-ionizer' formula [7].

The results of simulation show that increasing L is pointless, until the field penetration is changed. This is due to the fact that the ionizer volume can be divided into two parts. Only the part near the extraction opening is responsible for obtaining large efficiency. In the second part, not penetrated by the field, particles move randomly. Only the length of the second part increases with increasing L.

It was also shown that $V_{ext} = 1\,\mathrm{kV}$ is sufficient to obtain a satisfactory ionization efficiency.

Including other processes of ion production (e.g. ionization by fast electrons emitted from the ionizer wall, thermal ionization by particle collisions in the ionizer volume, etc.) to the presented model will be the aim of further investigation.

Acknowledgements

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