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IONIZATION EFFICIENCY CALCULATIONS FOR CAVITY THERMOIONIZATION ION SOURCE

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Турек М. и др. E13-2009-63
Расчеты эффективности ионизации
в термоионизационном ионном источнике

Описывается числовая модель ионизации в термоионизационном источнике ионов. Приводится обзор результатов расчетов эффективности ионизации для различных видов экстракционного поля. Также обсуждается зависимость эффективности ионизации от рабочих параметров, таких как длина ионизатора и экстракционное напряжение. Результаты численного моделирования сравниваются с теоретическими предсказаниями, полученными из упрощенной ионизационной модели.

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Ionization Efficiency Calculations for Cavity Thermoionization
Ion Source

The numerical model of ionization in a thermoionization ion source is presented. The review of ion source ionization efficiency calculation results for various kinds of extraction field is given. The dependence of ionization efficiency on working parameters like ionizer length and extraction voltage is disscused. Numerical simulations results are compared to theoretical predictions obtained from a simplified ionization model.

The investigation has been performed at the Dzhelepov Laboratory of Nuclear Problems, JINR and at the Institute of Physics, Maria Curie-Skłodowska University, Lublin (Poland).

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INTRODUCTION

Thermoionization ion sources of various design are widely used in electromagnetic isotope separation [1–5]. Their characteristic features are: high working temperature in the range 2500–3300 K and small dimensions of ionization chamber, also known as 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 thermoionization ion sources is their high ionization efficiency and small amount of substances needed to obtain stable ion current. Moreover, the time ions stay in ionizer volume is exceptionaly short.

The mentioned above advantages encouraged scientists to use thermoionization ion sources for on-line separation of micro-amounts of short-lived isotopes, which are created during irradiation of targets with high-energy proton beams.

The main part of thermoionization ion source (see Fig. 1) is cylindrical, semi-opened ionizer of length L and radius r. It is usually made of tungsten, molybdenum or tantalum — metals of high melting temperature. It is heated to the appropriate working temperature by electron beams from tungsten cathodes (usually two) K_1 and K_2. Ions are extracted from ionizer using extraction electrode on negative potential — U_{ext}. During on-line experiments the ionizer is simultaneosuly irradiated target, in which nuclear reactions induced by high-energy protons take place. Atoms — products of these reactions are ionized, extracted from the source, separated and after that guided to appropriate measurement set-ups, eg., gamma spectrometer.

Atoms produced in nuclear reactions inside the ionizer wall diffuse to ionizer's cavity. When they collide with hot walls of temperature T undergoes surface ionization with α probability given by the Saha–Langmuir equation [6, 7]:

$$\alpha = \frac{N^+}{N^a} = G \exp\left(-\frac{eV_i - \phi_e}{kT}\right), \tag{1}$$

where N^+ is the number of ions on the surface and N^a is the number of non-ionized atoms. The G coefficient is the constant characteristics of a given kind of atoms, V_i and ϕ_e are the ionization potential of atoms and the work function of the ionizer material, respectively. The α quantity is also known as ionization degree.

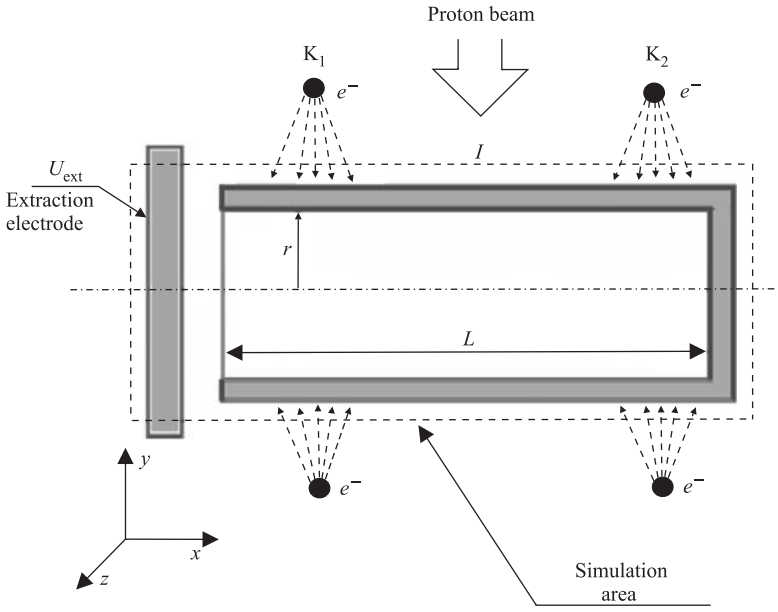

Fig. 1. The schematic view of thermoionization ion source. Simulation area is marked by dashed line rectangle

Another quantity describing ionization is the so-called ionization coefficient β given by

$$\beta = \frac{N^+}{N^+ + N^a} = \frac{\alpha}{1+\alpha}. \tag{2}$$

It should be stressed that defined above quantities describe single act of ionization. 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 atoms introduced into the ionizer N_0:

$$\beta_w = \frac{N^{+*}}{N_0}. \tag{3}$$

In our previous paper [8] the simple theoretical model of thermoionization ion source work was described. The model was based on assumption that atom touching hot ionizer surface is ionized with α probability and then desorbs moving in the direction determined by cosine angular distribution with respect to the normal. Two limiting cases were under investigation. In the first case the extraction field was neglected. Atoms and ions move in that case with constant velocity, along straight lines, until they hit ionizer wall or pass extraction opening.

Mean free path between collisions with walls were estimated. It enabled the division of the description into finite number of stages, at which particles remainig in ionizer volume are ionized/neutralized. In the second considered limiting case an assumption was made that extraction field inside the whole volume of ionizer is strong enough to remove every produced ion immediately after ionization. For such a working mode the source ionization efficiency calculated in the framework of discrete model by formula (9) in paper [8] may be much greater than β calculated from Saha–Langmuir formula. In practice such a work regime is very difficult to maintain mostly due to the necessity of very hight extraction voltage usage, e.g., for an ionizer of $L = 30$ mm, $r = 1$ mm and $T = 3000$ K one can estimate the necessary field strength as larger than 400 V/cm.

The aim of this paper is calculation of thermoionization ion source efficiency for more realistic working conditions, when the extractin field penetrates the ionizer 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 some large enough extraction voltage U_{ext} would lead to «each ion» working regime in the limited volume of the ionizer. It could allow obtainig ionization efficiency exceeding β. Simulation results will be compared to theoretical predictions. Simulations have been performed for various values of L (its radius was kept constant) in order to check the influece of ionizer elongation on ionization efficiency. The changes of efficiency due to the changes of extraction voltage were also investigated. For test and comparison reasons simulation of «each ion» working regime were done by assuming homogeneous extraction field in the whole volume of the ionizer cavity.

THE NUMERICAL MODEL

The Monte Carlo method based code follows trajectories of particles in the ionizer cavity. Near to the extraction opening there is a flat extraction electrode on the potential V_{ext} with respect to the ionizer. The distance between the electrode and extraction opening is 2 mm. The electrostatic field from the electrode penetrates the ionizer volume and influences the trajectories of ions. The «artificial» field may be also set in the code, e.g., homogeneous field directed along the ionizer axis. The simulation area, marked in Fig. 1, has been discretized using three-dimensional Carthesian spatial grid. The dimensions of the grid cells are $\Delta x = 0.2$ mm and $\Delta y = \Delta z = 0.1$ mm. The spatial grid has 100 cells in y and z direction, its size in x direction depends on ionizer length L. The electrostatic potential for particular boundary conditions is calculated by solving the Laplace equation

$$\Delta V(x, y, z) = 0. \tag{4}$$

The shape and potential values of extraction electrode and ionizer are set in some initial data file. Succesive over-relaxation technique [10] is used for solving the Laplace equation. The electrostatic field strenght values in grid nodes are worked out by numerical differentiation of potential, using the equation

$$\vec{E}(x, y, z) = -\vec{\nabla} V(x, y, z).$$

Particles are emitted from internal surface of the ionizer chamber according to cosine distribution function of their initial velocity direction with respect to the normal. The values of initial velocities correspond to the ionizer temperature $T = 2500$ K. Neutral particles move with constant velocity. The trajectories of ions are influenced by electrostatic field. The equations of motion are numerically solved using the standard 4th order Runge–Kutta method [10]. The values of electrostatic field strenght in the particle position are calculated by linear interpolation of corresponding values in neighbouring nodes. When the code detects that partilce hits the ionizer wall, Monte Carlo based subroutine decides whether the particle is ionized/neutralized or not, according to β parameter. The new initial velocity is determined and particle continues its journey until it leaves the ionizer. The code counts ions and neutral atoms leaving the ionizer and calculates ionization efficiency.

SIMULATION RESULTS

At the initial stage test simulation of the ion source work for the case of no extraction field has been performed. Simulations were done with an ensemble of 10^5 particles introduced into ionizer cavity. The dependence of the source ionization efficiency on ionization coefficient β was investigated for the ionizer of length $L = 8$ cm and radius $r = 0.4$ cm. The value of β coefficient changed in the range from 0.01 to 1. The lowest line in Fig. 2 represents the dependence obtained from simulations. It pertfectly matches theoretically deduced dependence $\beta_w = \beta$.

Next, homogeneous extraction field directed along ionizer axis (x axis) was assumed. Calculations have been done for field strength up to $E_0 = 5000$ V/m. Results are also presented in Fig. 2. It is easy to see that even the relatively weak field of $E_0 = 50$ V/m causes a remarkable increase of source efficiency. The use of stronger field leads to rapid increase of source efficiency, especially well visible for small values of β. The increase of field strength makes the $\beta_w(\beta)$ curves to tend to the $\beta_w = 1$ line.

The influence of field strenght on the number of particle collisions with ionizer walls (untill it passes the extraction opening) was also studied. Figure 3 presents probabilities $P(n)$ of leaving ionizer after n hits. Results were obtained for $\beta = 0.5$ and different values of E_0. One can see that for $E_0 = 5000$ V/m

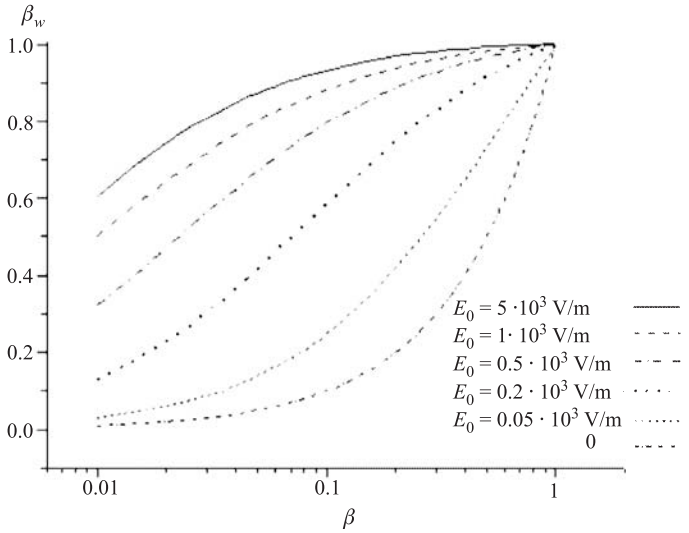

Fig. 2. Dependence of source ionization efficiency on β parameter in the case of homogeneous extraction field

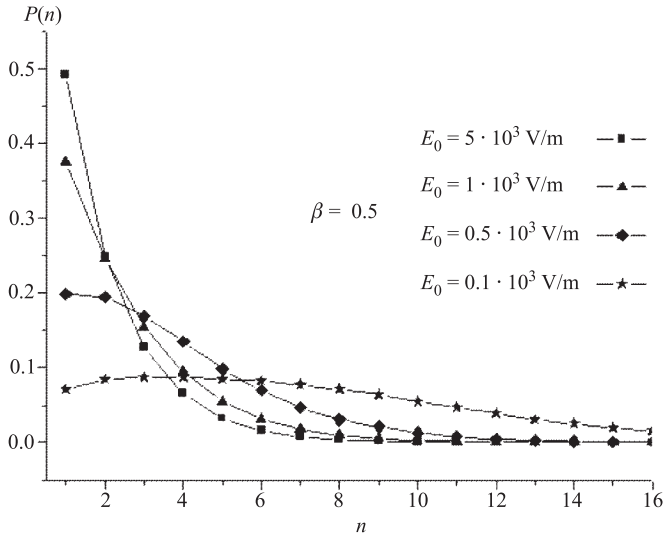

Fig. 3. Probability of leaving the ionizer by particle after n hits for different values of homogeneous extraction field strength

the ion source works very close to «each ion» regime — one half of particles leaves the ionizer after the first collision with wall (and ionization), one fourth after the second collision, etc. For smaller strength of the extraction field the mean number of collisions before passing the extraction opening increases: e.g., for $E_0 = 200$ V/m it is approximately 5 collisions with wall. However, even in the case of weak field, when the source does not work in the «each ion» regime, the increase of ionization efficiency is remarkable.

The change of ionization efficiency due to the increasing elongation of the ionizer was also under investigation. Simulations were carried out for $E_0 = 1000$ V/m and various L values. Results are shown in Fig. 4. It could be seen that the smaller is β of ionized substance, the larger is the influence of ionizer length. In the case of $\beta = 0.01$ an elongation of the ionizer from 2 to 4 cm yields in increase of efficiency twice as much. However, further increase of L up to 8 or 16 cm leads to relatively small effects. It should be noted that for large values of β effects due to the ionizer elongation are of minor importance.

After the analysis of limiting modes of ionizer work the more realistic model was considered. In this case the electrostatic field is an effect of the potential $U_{\rm ext}$ of the flat extraction electrode. The extraction field penetrates the ionizer volume at some distance. Its strenght decreases fast with the distance from the extraction opening. Figure 5 shows potential profiles along ionizer axis for different values

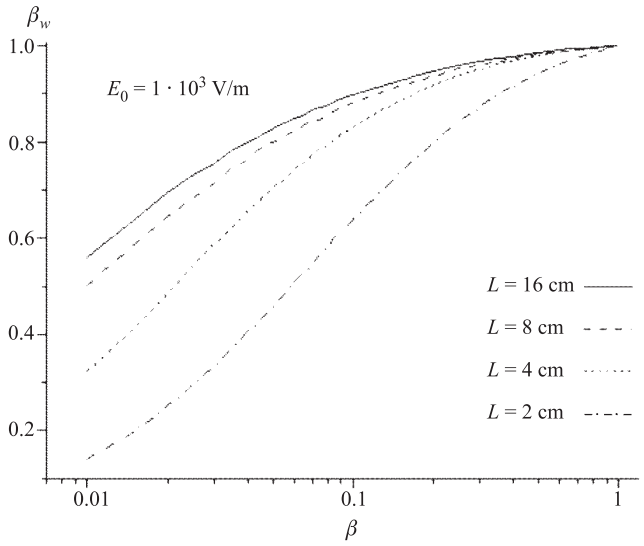

Fig. 4. Dependence of ionization efficiency on β parameter for different values of ionizer length in the case of homogeneous extraction field

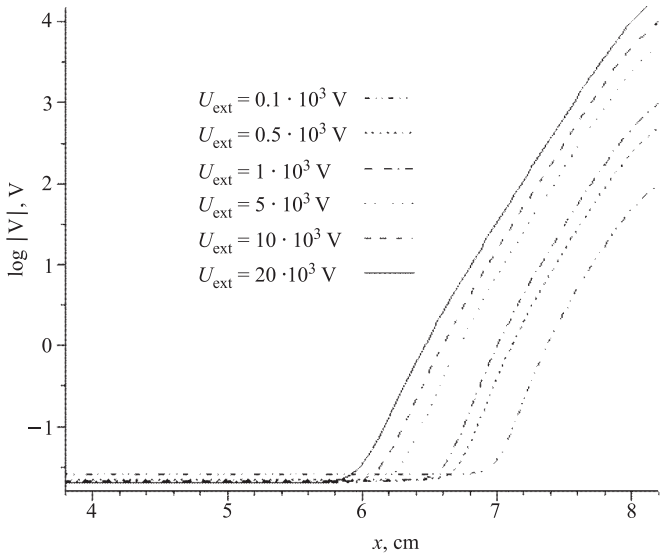

Fig. 5. Potential profiles along the ionizer axis in the case of realistic extraction field (note the logarithmic scale)

of extraction voltage. Calculations were done for ionizer of length $L = 8$ cm and radius $r = 0.4$ cm. For the case of $U_{\rm ext} = 100$ V the penetration depth is approximately 1 cm and it increases only to 2 cm for very large extraction voltage $U_{\rm ext} = 20000$ V.

The region penetrated by extraction field is crucial for obtaining larger ionization efficiency. Particles which are moving far from extraction opening does not feel the extraction field and roam inside the ionizer changing direction of motion randomly during collisions with ionizer walls. On the other hand, when charged particle reach (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. The results can be seen in Fig. 6 that presents dependence of ionization efficiency on β for different values of extraction voltage. Even very small value of extraction voltage $U_{\rm ext} = 100$ V gives quite satisfactory increase of β_w efficiency compared to the «no field» case. For substances of $\beta = 0.02$ the ionization efficiency grows four times for such small extraction voltage. One could expect that further increase of extraction voltage would lead to dramaticaly larger efficiency. But it is not the truth, as can be seen in Fig. 7, which shows the changes of efficiency β_w caused by extraction voltage. Small increase, approximately 25%, for substances of relatively small $\beta = 0.2$ could be observed when extraction voltage changes

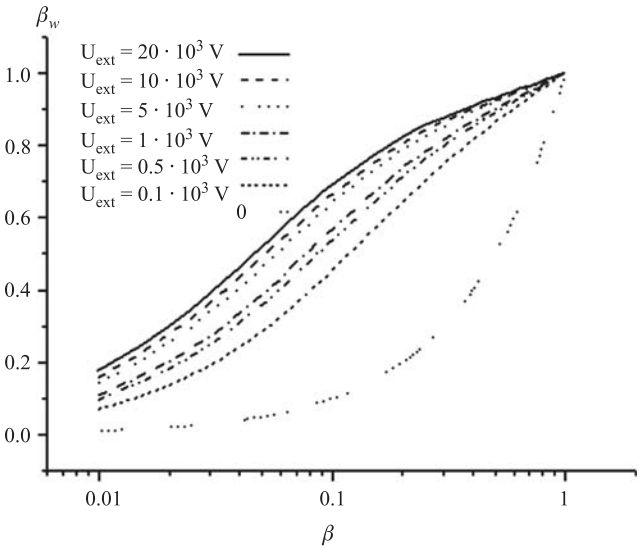

Fig. 6. Dependence of ionization efficiency on β parameter in the case of realistic extraction field

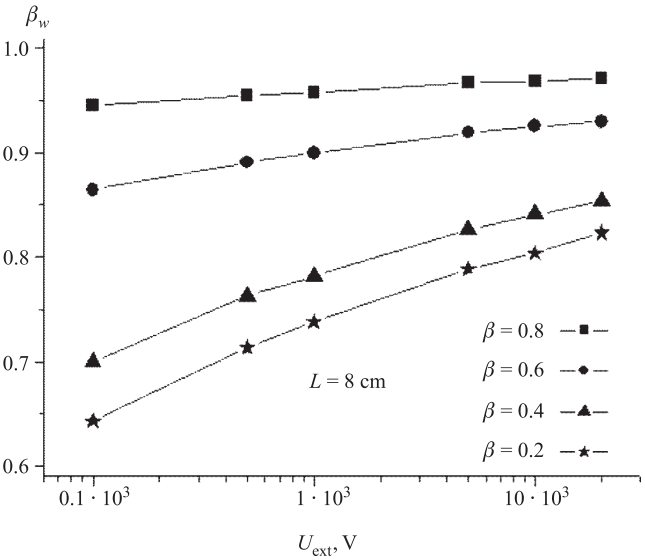

Fig. 7. Ionization efficiency as a function of extraction voltage $U_{\rm ext}$ in the case of realistic extraction field

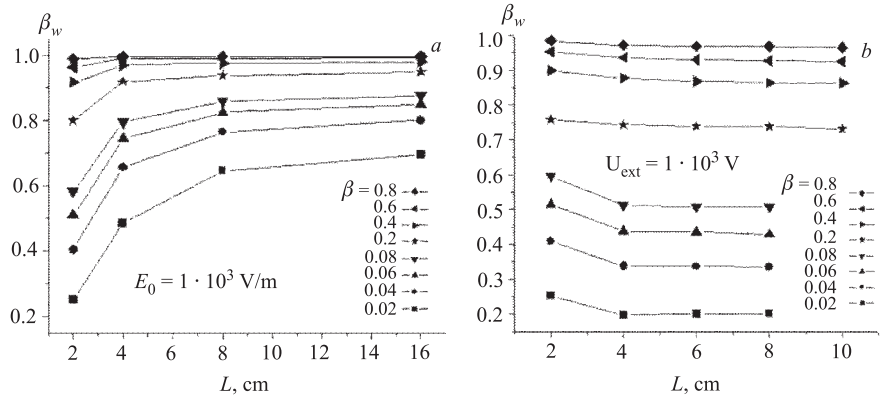

Fig. 8. Ionization efficiency as a function of ionizer length L in the cases of homogeneous (*a*) and realistic (*b*) extraction field

from $U_{\rm ext} = 100$ V to $U_{\rm ext} = 10000$ V. Hence, the excessive increase of extraction voltage is pointless, especially when one takes into consideration technical difficulties. Extraction voltage up to few thousand of volts are sufficient to obtain reasonable efficiency.

Figure 8.*a*, shows the dependence of $\beta_w(\beta)$ on ionizer length L for the previously considered case of homogeneous extraction field. As was previously said, one can see the increase of ionization efficiency with L, especially for small values of β. The longer is the ionizer, the longer particle travels toward extraction opening, the larger is probability of ionization.

On the other hand, in the case of realistic extraction field the large elongation of the ionizer does not seem to be desirable. It could be seen in Fig. 8, *b*. One can observe slight decrease of ionization efficiency when L grows. It can be understood when one have in mind that extraction field enters the ionizer at the depth of approximately 1 cm. The increase of ionizer length leads to elongation of «no extraction» region, where particles roam until they get close enough to extraction opening.

CONCLUSIONS

The numerical model of thermoemission ion source described in the paper enables much more realistic description than that presented in our previous paper [8]. Using computer simulations the calculations of ionization efficiency were done for limiting work regimes described in that paper. In the case without

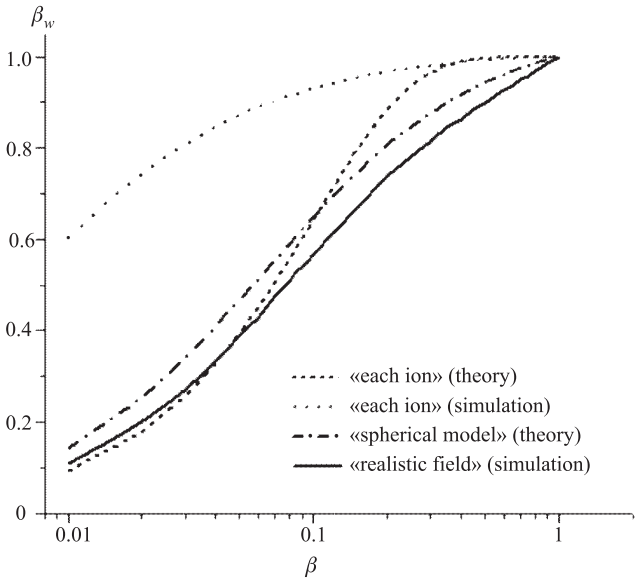

Fig. 9. Source ionization efficiencies $\beta_w(\beta)$ obtained from simulations as compared with predicted by theoretical formulae. Cases of «each ion» regime, $E_0 = 5000$ V/m (dotted line), «each ion» formula (9) from the paper [8] (dashed line), realistic field simulations with $U_{\rm ext} = 1000$ V (solid line) and spherical ionizer formula (15) from paper [8] (dash-dotted line)

extraction field simulations provide the same dependence $\beta_w = \beta$ as simple theoretical model. The «each ion» formula (9) from [8] describes very good $\beta_w(\beta)$ dependence for «each ion» simulations with homogeneous $E_0 = 5000$ V/m field for β greater than 0.3, as can be seen in Fig. 9. The simplifying assumption of the theoreticla model that non-charged particles drift toward extraction opening could be the reason of dicrepancies for smaller β values. In real ionizer, and also in simulations, neutral particles roam randomly inside the ionizer.

Simulations were also done for the realistic shape of extraction field. It should be noticed that the simulation results in this case are similar to those predicted by formula (15) from the paper [8]. The trends of both curves presented also in Fig. 9 are almost the same. The discrepancies may be caused by an assumption of spherical ionizer shape, which was made in [8].

In the case of realistic extraction field the ionizer volume could be divided into two parts. In the part near to the extractin opening the ionizer works in the mode near to the «each ion» regime. That is the part responsible for obtaining large source efficiency. The second part of the ionizer is not penetrated by extraction

field, in that region particles move randomly. Untill the field penetration depth is unchanged, the increase of ionizer length is pointless. Results of calculations for different $U_{\rm ext}$ values show that extraction voltages $U_{\rm ext} = 1000$ V are sufficient to obtain satisfactory ionization efficiency, provided the extraction electrode is close enough to extraction opening.

The model presented in the paper does not take into account any ion creation processes except surface ionization. The other possible mechanisms of ion production are, e.g., ionization by fast electrons emitted from ionizer wall, thermal ionization by particle–particle collisions in the ionizer volume, etc. Including of these processes to the presented model will be the aim of further investigation.

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