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Ionization of Short-Lived Isotopes in Spherical Hot Cavities

M. $TUREK^*$

Institute of Physics, Maria Curie Skłodowska University, pl. M. Curie-Skłodowskiej 1, 20-031 Lublin, Poland

The numerical model of ionization of short-lived nuclides in spherical hot cavities is presented. Two different cavity configurations are considered: one of them (the hemispherical one) resembles that known from already existing ion sources while the other (closer to the full sphere) could be more efficient for short-lived isotopes. Changes of ionization efficiency with the half-life period as well as with the particle average sticking time are presented and discussed. Influence of the extraction opening radius on ionization efficiency is also under investigation.

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1. Introduction

Hot cavity ion sources, invented in early 1970s [1, 2], are still employed, especially in the field of nuclear spectroscopy. They are still developed and optimized [3–6], mostly due to some strong advantages like: robust construction, high purity of the obtained ion beam, relatively high ionization efficiency and the fact that they need micro-amounts of the substance to be ionized. Another feature of that kind of ion sources is rather short time a particle stays in the ionizer, which could be crucial during the studies on short-lived isotopes [7, 8].

The most important part of the considered kind of ion source is an ionizer with a cavity. It could be elongated, e.g. having a form of a tube, however, more compact spherical ionizers are also used [9–11]. The ionizer is heated to high working temperatures (≈ 2000 K or more). It could be also a target irradiated in order to produce nuclides that are to be ionized [12], otherwise it has to be connected to the target via some kind of a transfer tube [13].

Atoms in the cavity are adsorbed at a hot wall (or diffused out of the ionizer wall bulk) and ionized with the probability given by the Saha–Langmuir formula. The ionization degree, i.e. the rate of ions and neutrals is

$$\alpha = G \exp\left(-\left(V_{\rm i} - \varphi_{\rm e}\right)/kT\right),\tag{1}$$

where V_i and φ_e are the ionization potential of an atom and the work function of the ionizer material, respectively. The *G* coefficient depends on the atom/surface combination. In order to keep formula (1) valid for negative ion production, one has to substitute $V_i - \varphi_e$ with $\varphi_e - E_a$, where E_a is the electron affinity. The other useful quantity is the ionization probability in a single act, which could be calculated as

$$\beta = \alpha / (1 + \alpha) \,. \tag{2}$$

Particles undergo many (even thousands) collisions with hot walls, which lead to ion source efficiency (understood as the ratio of the number of obtained ions to the number of all particles introduced into the cavity) much higher than that predicted by Eq. (1). Numerous theoretical approaches [14–17] tried to describe this phenomenon. A relatively less effort was made creating numerical models of the transport and ionization in hot cavities [18, 19].

In the previous papers [20, 21] the ionization of shortlived isotopes mostly in tubular ionizers was considered. Ionization of stable nuclides in spherical cavities was also studied. The aim of the current paper is investigation of ionization of short-lived nuclides in the spherical hot cavity ion sources. The numerical model, extended in order to implement such cavity shapes in a way similar to the case of stable isotopes [22], is briefly presented. Two kinds of the cavity configurations are considered in the paper: one of them is almost a full sphere with a small extraction opening, while the other one is a hemisphere with a flat endcap. Changes of ionization efficiency with the nuclide half-life period are investigated for both configurations. Influence of the average particle sticking time on the total time a particle stays inside the ionizer as well as on the ionization efficiency is discussed. Dependences of ionization efficiency on the size of the extraction opening calculated for both configurations are compared.

2. Numerical model

Numerical model of ionization is similar to that described in [20, 21, 23–25] where mainly tubular ionizers were considered. In the paper spherical ionizers are under investigation. Figure 1 shows the schematic view of the simulated system. For the sake of simplicity, a flat extraction electrode on the negative potential $-V_{\rm ext}$ is used. The simulation area is covered by a three-dimensional mesh (500 × 100 × 100 cells). The cell sizes are: $\Delta x = 0.1$ mm, $\Delta y = \Delta z = 0.05$ mm.

It is assumed that each particle undergoes ionization/neutralization when touching the hot inner surface of the cavity according to the probability described by Eqs. (1) and (2). Moreover, a particle stays at the surface for some period of time, which is determined using a standard Monte Carlo approach for each collision

$$t_{\rm stick} = -\tau_{\rm s} \ln {\rm RND}, \qquad (3)$$

where τ_s is the average sticking time and RND is a normal pseudorandom number. Typical values of τ_s are given e.g.

^{*}e-mail: mturek@kft.umcs.lublin.pl



Fig. 1. The geometry of the simulated hot cavity ion source.

in [26]. After overcoming the potential barrier at the hot surface, the particle travels inside the cavity with the initial velocity corresponding to the surface temperature and a random distribution of the velocity vector direction. The equations of motion are solved numerically. Electric field is calculated by numerical derivation of the electrostatic potential $\boldsymbol{E} = -\boldsymbol{\nabla}V(r)$. The potential is found by solving the Laplace equation with the boundary conditions determined by electrode shapes and voltages. Successive over-relaxation technique is used as in [27– 31]. As the pressure in the cavity is usually very low (below 10^{-4} mbar), collisions with other particles could be neglected. The model takes into account radioactive decay of nuclides. The primary nuclide decays after the time $\tau_{\rm dec}$, which is calculated according to the formula

$$t_{\rm dec} = -\tau_{1/2} \ln \text{RND},\tag{4}$$

where $\tau_{1/2}$ is the half-life period. The code follows trajectories of particles until they pass the extraction opening and counts the number of ions of primary and secondary nuclides ($N_{\rm p+}$ and $N_{\rm s+}$) as well as that of neutrals ($N_{\rm p0}$ and $N_{\rm s0}$). The ion source ionization efficiency is defined as the ratio:

$$\beta_{\rm s} = \frac{N_{\rm p+}}{N_{\rm p+} + N_{\rm s+} + N_{\rm p0} + N_{\rm s0}}.$$
(5)

3. Results and discussion

Two different shapes of ionizer cavity were considered. First of them (A), introduced in [22], is a spherical cavity with a small extraction hole. Such a shape results in an increase of the total ionization efficiency due to numerous collisions with cavity hot walls. The radii of the cavity aperture r_1 as well as the extraction opening in the flat endcap r_2 are the same ($r_1 = r_2 = 0.5$ mm) and smaller than the inner radius of the cavity $r_{\rm ion} = 2$ mm. The second configuration (B) resembles much shapes of the ionizers widely used in several ion sources [9–11]. It could be defined by the choice $r_1 = 0.5r_{\rm ion}$ and $r_2 < r_1$. As in the previous case $r_{\rm ion} = 2$ mm and $r_2 = 0.5$ mm were chosen. In both cases the flat extraction electrode ($V_{\rm ext} = -2$ kV) was placed at the distance d = 2 mm from the extraction opening.

Changes of the ionization efficiency with the half-life of the primary nuclide for the two configurations were studied at first. Calculations were done using 200000 particles of mass 150 a.m.u. The simulation time step was 10^{-8} s. The ionizer temperature was set as kT = 0.31 eV. The values of the nuclide half-life period changed in the range 0.1 s-0.001 ms. As in the case of tubular ionizers [20, 21] one can observe (see Fig. 2) deterioration of ion source efficiency with the decreasing $\tau_{1/2}$. However, it is worth noticing that even for very small values of β (0.005) and $\tau_{1/2} = 1$ ms the ionization efficiency in the case of spherical ionizers is almost of order of magnitude higher than that obtained for the tubular ones. This is mainly due to the compact shape of the spherical or hemispherical cavities, leading to shorter times a particle stays inside the ionizer (in the case of $\tau_s = 0$): 0.7 ms for the tubular ionizer [20, 21] while 0.4 ms for the configuration A and 0.2 ms only for the configuration B (see Fig. 2c). Ionization efficiency in the case of small β is approximately 30-40% higher for the configuration A compared to that in the case of configuration B. This is most probably due to the larger area of hot ionizer surface. The configuration A is also favourable for larger values of ionization coefficients — compare the convex shape of $\beta_{s}(\beta)$ curves obtained for the configuration A with the concave ones of the curves calculated for the configuration B. This could be understood as the effect of ion losses during the collision with the colder surface of the flat endcap.



Fig. 2. Ionization efficiency as the function of β for different half-life periods calculated for the configurations: A (a) and B (b). Average time a particle stays in the ionizer (c) for $\tau_s = 0$.

The supremacy of configuration A is also confirmed by the simulation results shown in Fig. 3a and b. They present the influence of the average sticking time on the ionization efficiency. The half-life $\tau_{1/2} = 0.01$ s was chosen while $\tau_{\rm s}$ changed in the range 0.01 s down to 1 μ s.



Fig. 3. Ionization efficiency as the function of β for different values of average sticking time for the configurations: A (a) and B (b). Average time a particle stays in the ionizer (c) and (d).

All other parameters were kept the same as in the previous case. As particles undergo more than one hundred collisions (on average) with the cavity wall, the lowering of $\beta_s(\beta)$ curves is observed for both configurations. The configuration A is at least by 30% more efficient than B (note that for $\beta < 0.1$ the efficiency for B increases much more slowly than for A). The difference of efficiencies could be explained by the fact that the average times $\langle t \rangle$ are larger for the configuration B, as can be seen in Fig. 3a and b. This is most probably due to the larger number of collisions on the way to the extraction opening (including non-ionizing collisions with the endcap). It should be also noticed that the decrease of $\langle t \rangle$ with β is much faster in the case A, which results in convex shape of $\beta_s(\beta)$ curves and higher efficiency.



Fig. 4. Changes of the ionization efficiency with the size of the extraction opening for both configurations.

The changes of ionization efficiency with the size of the extraction opening were also under investigation. Simulations were done for r_2 changing in the range from 0.25 mm up to 1 mm. The results are shown in Fig. 4. The optimal efficiency is achieved for approximately $r_2 = 0.7$ mm for the configuration A. The saturation of $\beta_s(r_2)$ curves is observed for higher values. On the other hand, one observes rather rapid decrease of $\beta_s(r_2)$ curve inclination in the case B. The $\beta_s(r_2)$ curves could be divided into two parts: the one corresponding to the fast increase of β_s , for $r_2 < 4$ mm and the other, showing constant but rather slow growth of β_s with r_2 . Despite this tendency, one should keep in mind that efficiency (in the saturation range) of the configuration A is approximately 70% higher than that of the configurtion B. These ratios are similar for all considered $\tau_{1/2}$. In both cases one may assume that above some r_2 , the extraction field is able to catch ions soon after they appear, and no further increase of r_2 is necessary.

4. Conclusions

The numerical model of hot cavity ion source was upgraded in order to describe ionization of short-lived isotopes in spherical ionizers. Changes of ionization efficiency with the nuclide half-life period and the average sticking time were calculated and discussed for two different ionizer geometries. It was shown that the proposed spherically shaped ionizers could be much more efficient than the tubular ones for short-lived isotopes, mostly due to their compact shape, leading to shorter times a particle stays in the cavity. It was also found that the efficiency of the fully spherical ionizer is 30-70% higher than that of the hemispherical ionizer, employed in some ion sources. Simulations for different radii of the extraction opening r_2 suggest that in both considered cases the ionization efficiency increases fast with r_2 up to a certain level only.

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