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Ionization Efficiency in a Hot Flat Disc-Shaped Cavity

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Abstract

Hot cavity ion sources of different kinds are widely used in nuclear and mass spectroscopy, especially in on-line isotope separation devices attracting attention of scientists and engineers looking for high ionization efficiency, robustness and beam purity. In the paper a new type of hot ionizer cavity is proposed: namely cavity having the shape of a flat disc, which may be especially suitable for short-lived nuclides to be ionized.

A numerical model of the ion source is presented in the paper. The particle tracking code takes into account ionization at hot surfaces and enables modeling of both flat disc cavity and standard elongated cavity ionizers. The code enables calculation of total ionization efficiency and is suitable for stable and long-lived nuclides.

Influence of the flat disc cavity geometry (thickness and radius) and its temperature on total ionization efficiency was considered – it was shown that the efficiency increases with cavity radius due to the growing number of particle-wall collisions. This effect may be important in the case of the hard-to-ionize nuclides.

The optimal ionizer geometry is characterized by 90 % efficiency, even for substances with rather low ionization coefficient (of order 0.05). The role played by the size of the extraction opening is explained – it is demonstrated that the ionization efficiency increases due to the opening radius reduction. It is also proven that extraction voltage of 1–2 kV is sufficient to maintain optimal ionizer efficiency.

Keywords: ionizer, ionization efficiency, cavity, extraction opening.

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Эффективность ионизации в горячей плоской дискообразной полости

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Ионизаторы с горячей полостью различного типа находят широкое применение в атомной и масс-спектроскопии, в частности, в устройствах для разделения изотопов в режиме онлайн, представляют большой интерес для учёных и инженеров вследствие высокой эффективности ионизации, надёжности и чистоты луча. В работе предложен новый тип горячей ионизационной полости, а именно полости в форме плоского диска, особенно эффективной для ионизации короткоживущих нуклидов.

Представлена численная модель ионного источника. Модель отслеживания частиц учитывает ионизацию на горячих поверхностях и позволяет моделировать как полость плоского диска, так и стандартные ионизаторы с удлинённой полостью. Модель позволяет выполнять расчёт общей эффективности ионизации и применима к стабильным и долгоживущим нуклидам.

Рассмотрено влияние геометрии полости плоского диска (толщина и радиус) и его температуры на общую эффективность ионизации – показано, что эффективность увеличивается с радиусом полости из-за растущего числа столкновений частиц со стенками. Данный эффект может оказаться важен для трудноионизируемых нуклидов.

Оптимальная геометрия ионизатора характеризуется эффективностью 90 % даже для трудноионизируемых веществ с коэффициентом ионизации порядка 0,05. Объясняется роль, которую играет размер экстракционного отверстия – показано, что эффективность ионизации увеличивается из-за уменьшения радиуса отверстия. Также доказано, что выходное напряжение 1–2 кВ достаточно для поддержания оптимальной эффективности.

Ключевые слова: ионизатор, эффективность ионизации, полость, экстракционное отверстие.

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Introduction

Surface ionization ion sources equipped with hot cavities proved to be useful tools e.g. in nuclear spectroscopy [1], mass spectroscopy [2, 3] and are widely used in on-line isotope separation (ISOL) projects [4–7]. Hot cavity ion sources in its pure form were invented almost five decades ago [8, 9] and evolved into the resonant ionization laser ion sources (RILIS) [10–12] based on an excitation of the valence electron to the continuum by tunable lasers. It is worth mentioning that the evolution has not stopped and next hybrid ion sources for ISOL purposes still appear [13]. Numerous advantages of hot cavity ion sources like: compact design, robustness and reliability, very low energy spread of the ion beam and its high purity and, probably most of all, high efficiency and very small amounts of ionized substance needed to obtain a good quality ion beam made these devices attractive to physicist and engineers.

There is a variety of hot cavity ion sources, but in their classical form the basic part is a semi-opened ionizer made of refractory metal or ceramics, heated to a high working temperature (≈ 2500 K or more) either by electron beams [14] or ohmically [15, 16] or even inductively [17]. Most often the ionizer is connected to a target irradiated in order to produce isotopes by a kind of transfer line [18], but in some solutions the ionizer itself could serve as the target and the produced isotopes are released immediately into the hot cavity [14]. As it has been already said, the cylindrical ionizer is the most common solution, but spherical ones are also used in some devices [19, 20].

In a series of previous papers a numerical models of a variety of hot cavity ion source were presented, including those concerning tubular [21–23], spherical or hemispherical [24] and also conical ionizers [25]. Results presented by other groups also showed that ionizer of complex shapes are characterized by very high efficiencies [26, 27]. At the early version of the model ionization of stable isotopes was considered, later on the model was upgraded in order to take into account effects of radioactive decay and delays of the particle emission due to diffusion and effusion in the ionizer [28]. The ionization model is based on the assumption that multiple collisions of particles with hot ionizer walls enhance total ionization efficiency. It should be mentioned here that e.g. electron impact ionization could also provide very important contribution, especially in the case of hard-to-ionize elements [22].

As it has been said before, geometry of the ionizer cavity may be crucial for obtaining high ionization efficiency. It was e. g. demonstrated that spherical ionizers with small extraction openings achieve higher efficiency than tubular semi-opened ionizers in the case stable nuclides, while in the case of short-lived isotopes either hemispherical or conical ionizers are superb. In the current paper another shape of the ionizer is postulated. It is a flat disc cavity ionizer, which could be understood as a limiting case of cylindrical ionizer, but characterized by shorter length compared to its radius. The flat shape of the cavity should result in a large number of collisions of the particle traveling to the extraction opening. Simultaneously, small length of the cavity makes the penetration of the extraction field easier, leading to fast and effective ion evacuation. It should be also mentioned that manufacturing of the flat disc cavity seems to be easier task than in the case of spherical or even conical cavities, especially in the case of hard-to-machine materials. The paper contains brief description of the numerical model suitable for stable and very long-lived isotopes. Dependency of the ionization efficiency on the cavity shape (its elongation an radius) is studied. The influence of the extraction opening size on the efficiency is under consideration. The current-voltage curves obtained for different values of ionization coefficient are also presented and discussed. The changes of the ion yield due the ionizer temperature are investigated.

Numerical model

The numerical code used for calculation of ionization efficiency in a disc cavity is a trajectory tracking code similar to that considered in previous papers [21–25, 28]. The code follows trajectories of both ions and neutral particles that are confined in a hot cavity until they reach the extraction opening. A schematic cross-section through the simulated cavity-extraction electrode system is presented in Figure 1.

It should be stressed once again that standard cylindrical ionizer is characterized by $r_i << L$ condition, whilst for a flat disc cavity L should be much smaller or at least comparable to r_i. The results presented in the paper were obtained for L of order of 1 mm. The simulation system is discretized using by $100 \times 400 \times 400$ rectangular numerical mesh with cell sizes $\Delta x = \Delta y = \Delta z = 0.05$ mm. The electrostatic potential is worked out by numerical solving of Laplace equation (with boundary condition imposed by electrodes) employing the successive over-relaxation method, as in [29, 30]. The classical equations of motion are integrated using 4th order Runge–Kutta algorithm. The forces used by the push subroutine are found by linear interpolation of the electric field values at six nodes nearest to the particle position. Starting velocities of particles depend on the ionizer temperature, while their initial directions are chosen randomly. A neutral particle or ion that hits the ionizer's hot internal surface could undergo ionization/neutralization with a probability (also called ionization coefficient) β, which is related to ionization degree by formula:

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

The latter magnitude (α) is usually defined as the ratio of the numbers of ions and neutral atoms detaching from the hot surface and could be estimated using the Saha–Langmuir formula:

$$\alpha = G\exp(-(V_i - \phi_e) / kT). \tag{2}$$

In the above formula V_i and ϕ_e are the ionization potential and the work function of the ionizer material, respectively, while the G prefactor depends e.g. on the atom-surface reflection coefficient. As it was already mentioned, the code follows the particles until they exit the cavity through the extraction hole and registers the total numbers of ions (N_+) and of neutrals (N_0). The total ion source ionization efficiency is calculated as:

$$\beta_s = \frac{N_+}{N_+ + N_0}. \tag{3}$$

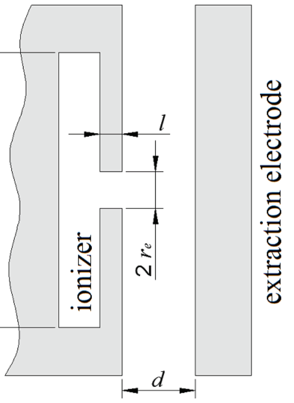


Figure 1 – Schematic view of the simulated system

One should have in mind that particles inside the cavity undergo many collisions with the ionizer hot walls. As the collision number reaches hundreds or even thousands, and charged particles are caught by the extraction field, the β_s could be by orders of magnitude larger than ionization probability during a single collision, predicted by the Saha–Langmuir formula (2).

Simulation results

The influence of ionizer cavity shape on ionization efficiency was investigated as the first. Namely, r_i radius was changed starting from 0.8 mm up to 7 mm while the ionizer length L was kept constant ($L = 1$ mm). The flat extraction electrode on potential $V_{ext} = -2$ kV) was set at the distance $d = 1$ mm from the extraction hole of radius $r_e = 0.5$ mm. The extraction channel length was chosen as $l = 0.2$, unless otherwise stated. The simulation timestep was chosen as 10–2 µs. Simulation runs were performed using 20000 test particles of 150 a.m.u. mass. The ionizer temperature was set to $kT = 0.3$ eV, unless otherwise stated. Calculation results are shown in Figure 2. As one can see, β coefficient changed over two and a half decades. Obtained total efficiency increases very fast with β. As one may expect ionization efficiency increases with the cavity radius and this effect is especially important in the case of hard-to-ionize substances (the case of β of order 0.01 or less). The total ionization efficiency could be several tens times larger than efficiency predicted by Saha–Langmuir law. For example, for β = 0.01 the total efficiency reaches 0.5 in the case of flat enough cavities ($r_i = 4$ mm or more). The 90 % efficiency, marked as a dotted horizontal line, could be achieved for β larger than 0.06, which is significantly better than efficiencies achieved in the case of cylindrical [21] and hemispherical ionizers and comparable to that reached in spherical ionizers [24]. As it was already mentioned, the efficiency gain is reached due to the increasing number of particle-wall collisions in the case of flat cavities. As one can see in Figure 2. the average number of collisions increase dramatically with r_i. For small values of β it reaches 700 in the case of very flat cavity while it is ≈ 30 for the compact shape. It could be seen that $<n_{hit}>$ decreases with β – the easier is an atom to be ionized, the faster is caught by the extraction field.

On the other hand, in a flat disc shaped cavity the volume that is far away from the extraction field increases very fast with the ionizer radius. Decreasing probability of ion extraction leads to the saturation of ionization efficiency growth with r_i. As it could be seen in Figure 3 an excessive increase of r_i – above 7 mm in the considered case – is pointless, as it will not result in efficiency improvement.

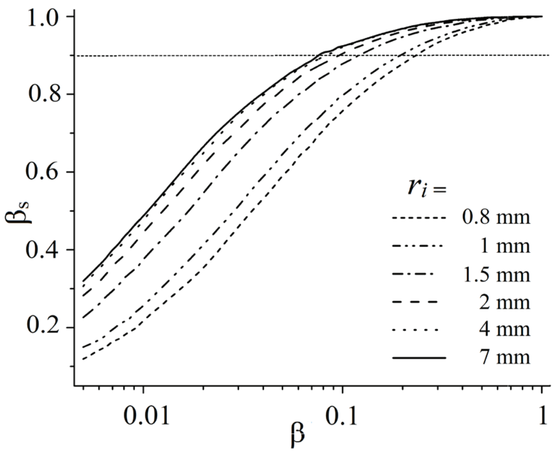


Figure 2 – Total ionization efficiency as a function of ionization coefficient β for different values of ionizer radius r_i

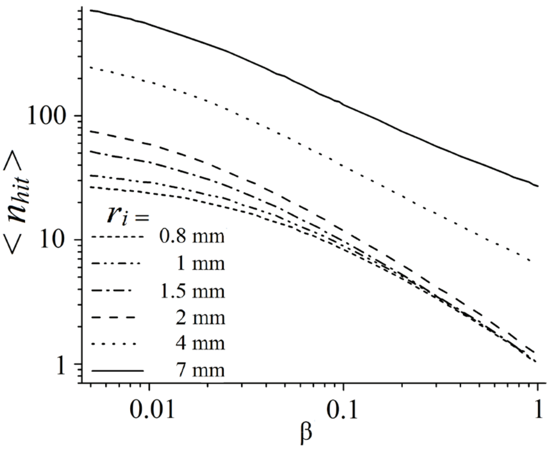


Figure 3 – Average number of particle-wall collisions calculated for different values of ionizer radius r_i

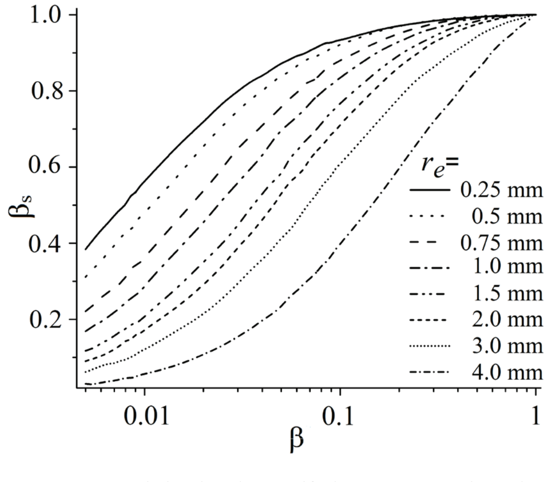


Figure 4 – Total ionization efficiency as a function of ionization coefficient β for different values of extraction opening radius r_e

The influence of extraction hole radius was also under investigation. Calculations were done for a disc cavity of diameter $r_i = 5$ mm and $L = 1$ mm. Results for re changing in the range from 0.25 mm up to 4 mm are presented in Figure 4. One can see that total ionization efficiency increases with r_e. Once again that effect is more important for smaller β. The explanation is very similar to that given in the previous case: the smaller is the extraction hole, the more collision with the hot wall each particle undergoes, which enlarges the total ionization probability. The average number of collisions as function of β is shown in Figure 5. The increase of the average number of collisions by three orders of magnitude when the extraction hole radius is reduced to 0.2 mm is meaningful. One should, however, have in mind that the presented results were obtained for stable isotopes. More particle-wall collisions result in longer total time a particle stays in the ionizer, which may play a crucial role in the case of short-lived isotopes.

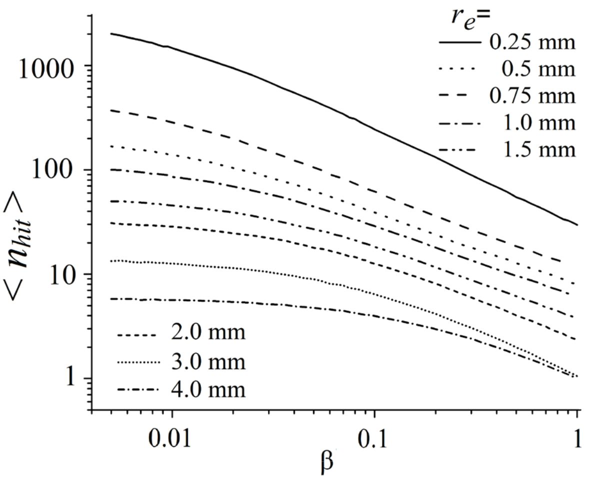


Figure 5 – Average number of particle-wall collisions calculated for different values of extraction opening radius r_e

The role played by the disc cavity thickness L was also checked out. Simulations were performed for $r_i = 2$ mm and $r_e = 0.05$ mm, all other parameters were as in the previous cases. The results are shown in Figure 6. One can see slight reduction of ionization efficiency for a very thin cavity ($L = 0.5$ mm). This could be probably due to the fact that the penetration of extraction field is limited in the case of such a flat cavity. For larger values of L the changes of efficiency are rather subtle, independently on the ionization coefficient.

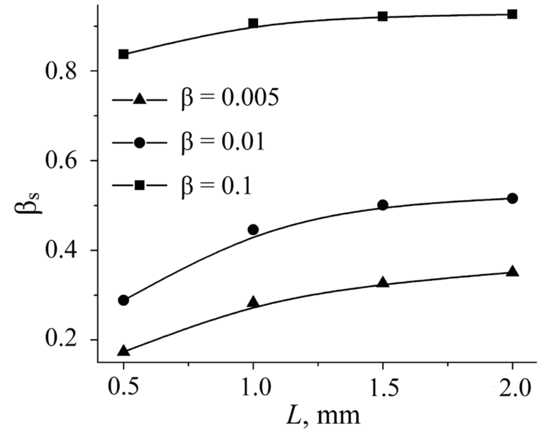
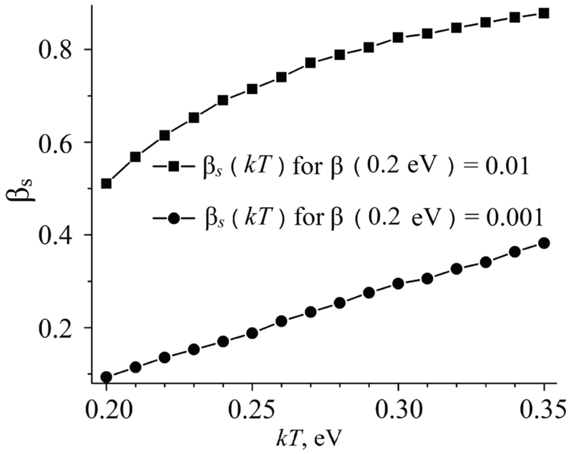
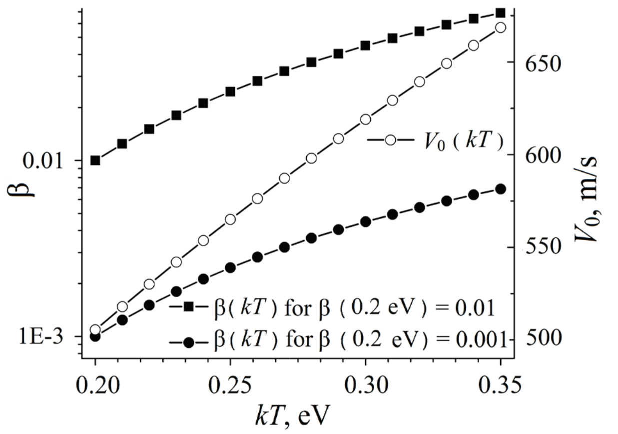


Figure 6 – Influence of disc-shaped cavity thickness L on the total ionization efficiency

Ionizer temperature may play an important role in achieving large ionization efficiencies. Figure 7 presents results of simulations of β_s evolution with kT for a flat disk cavity. Simulations were performed for $L = 1$ mm, $r_i = 5$ mm and $r_e = 0.5$ mm. Two cases were considered: ionization coefficient in the lowest considered temperature $kT = 0.2$ eV was set either to 0.01 or 0.001. Ionization coefficient for higher temperatures was calculated using Saha–Langmuir formula assuming V_i-$\phi_e = 0.9$ eV. Changes of ionization coefficient with kT are shown in Figure 7*b*. It could bee seen that β increases several times in the considered temperature range. This is not the only magnitude that changes with ionizer temperature. Hollow symbols show the dependence of the desorbing particle initial temperature on kT – that change was also taken into account by the code. As it is shown in Figure 7*a*, total ionization efficiency increases with kT. The increase is nearly linear for β(0.2 eV) = 0.001, while a kind of saturation could be expected in the cases of higher initial ionization coefficient β.



a



b

Figure 7 – Total ionization efficiency as a function of ionizer temperature kT (*a*) and dependence of ionization coefficient β and initial velocity of the desorbing particle on ionizer temperature kT (*b*)

As for other shapes of the ionizer, simulations of the current-voltage curves were done (see Figure 8).

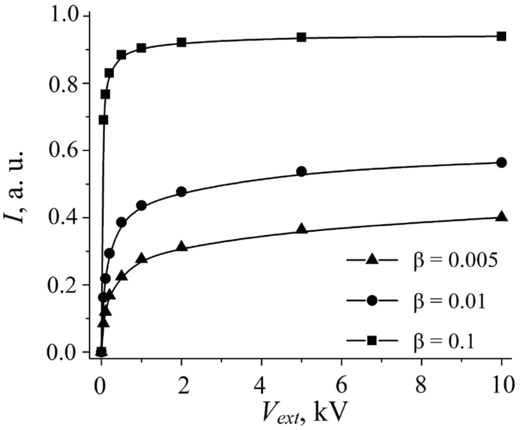


Figure 8 – Current-voltage curves calculated for different values of ionization coefficient β

The case of $L = 1$ mm, $r_i = 5$ mm and $r_e = 0.5$ mm was considered (the same set of parameters as previously). Extraction voltage was increased up to 20 kV. One can observe very rapid increase of ion current with V_{ext} rising up to ≈ 1 kV. Above 1–2 kV a saturation of current-voltage curve is observed. This happens when the extraction field is able to catch and extract ions almost immediately after they are created. It should be kept in mind that excessive (more than 1–2 keV in the considered case) increase of the V_{ext} is pointless – it does not lead to any significant increase of β_s and may result in electrical breakdown. It is worth noting that the shape of the calculated curves is close to that obtained for tubular [23, 28] ionizers and to experimental curves measured for the tubular ionizers [31].

Conclusion

Stable isotope ionization in a novel kind of hot cavity, namely flat disc-shaped one, was considered in the paper. The brief description of the numerical model was given for completeness. Influence of the ionizer geometry on ionization efficiency was considered. It was shown that the efficiency increases with the disc ionizer radius reaching values higher than these obtained for elongated cylindrical or hemispherical ionizer. Ionization efficiency of 90 % could be reached even in the cases of the ionization coefficient of order 0.05. This effect is mostly to the large number of particle-ionizer wall collisions (reaching several hundreds) in the case of flat cavities.

Numerical simulation performed using the model showed also that:

– ionization efficiency of stable isotopes could be significantly enhanced by the reduction of the extraction opening radius;

– excessive reduction of that thickness (below 0.5 mm) may lower the total ionization efficiency;

– extraction voltage of 1–2 kV is sufficient to achieve almost maximal efficiencies at given geometry.

Simulations of the influence of the ionizer temperature on the total ionization efficiency showed that the efficiency increases with kT, mostly due to the fact that ionization probability usually increases with the surface temperature. Thus, it is crucial to maintain possible high ionizer temperature (for typical ionization conditions) and reduce chances of forming "cold spots" that could reduce efficiency to a large extent.

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