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Spatial distributions of neutral atoms in the near-target plasma: Theory and experiment

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Abstract

In this paper analytical expressions are given for the distributions of neutral impurity atoms in the plasma near the surface, which acts as the impurity source. The effects of the angular and energy distribution of the sputtered atoms, of the experiment geometry (plasma and surface size) and the plasma parameters are taken into account. Using the analytical expressions and experimentally measured photon intensities of the neutral line emission, either the flux of eroded particles or the excitation rate coefficients can be determined experimentally, by knowing one of them. In the linear plasma generator PSI-1 such an experiment with Li, for which the excitation rate coefficients are available, has been performed. The measured flux of eroded Li atoms has been compared with erosion calculations taking into account both thermal sublimation and physical sputtering.

Keywords: Spatial neutral distribution; Analytical model; Plasma–wall interaction

1. Introduction

In fusion experiments, atoms eroded as neutrals from the plasma facing surfaces are released with a certain angular and energy distribution. They move along straight trajectories in the plasma until they become ionized. Only in the case where the neutrals are ionized near the source location the influx rate can be inferred simply from the measured line emission intensity integrated over the entire ionization/excitation region. In other situation where the optics do not collect all the photons or not all the atoms are ionized before leaving the observed space the knowledge about the spatial distribution of the neutrals is quite necessary. The spatial position of their ionisation depends on the initial energy, the plasma parameters and on the statistical nature of the ionization process itself. Having a source, i.e. the flux of eroded atoms and a loss term, i.e. the ionization, a steady state density distribution of the neutral impurities in front of the surface is established. Analytical expressions are given in Section 2 for these distributions in the near-target plasma for different angular and energy distributions of the sputtered particles. Furthermore, the effects of the probe and plasma geometry as well as the plasma parameters are taken into account. The spatial distribution of the sputtered neutral atoms can be obtained experimentally by measuring the line-of-sight photon intensities of the neutral line emission [1]. In order to relate the photon intensity to a local density of the neutral atoms the branching ratio for the certain observed spectral line and the excitation rate coefficient have to be known. However, for materials being of interest as plasma facing components in fusion devices (such as Be, C, W) these values are known only with large uncertainties. In well defined plasma experiments these coefficients can be defined by means of the derived analytical expressions giving below. If the excitation rate coefficients are known with a satisfactory accuracy the flux of eroded particles can be determined in these experiments. Such an experiment with Li has been performed in the linear plasma generator PSI-1 [2]. The experimental setup is described in Section 3. The measured distributions have been compared with those obtained by the theory (Section 4).

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2. Theory – Analytical model

Analytic expressions of the spatial distribution of neutrals have been derived in [3] for the case of a narrow beam injection of impurities. In the following such expressions are obtained if a surface acts as the impurity source and the angular distribution of the emitted particles has to be included into the consideration. The number of particles sputtered from a surface element dF during a time interval dt is $\Gamma \cdot dF \cdot dt$, where Γ is the flux of the sputtered atoms. Taking a cosine distribution as the angular distribution of the sputtering process [4] one obtains for the number of particles emitted into the solid angle $d\Omega$: $\Gamma \cdot dF \cdot dt(\cos\theta/\pi)d\Omega$, with θ being the angle with respect to the surface normal. During the same time interval dt the moving particles form the volume $d\Omega \cdot r^2 \cdot dr = d\Omega \cdot r^2 \cdot v\,dt$ where v is the velocity of the sputtered particles. Following, the neutral density $n(r, \theta)$ can be calculated as:

$$n(r,\theta) = \frac{\Gamma\, dF\, dt \cos\theta\, d\Omega}{\pi r^2 v\, dt\, d\Omega} = \frac{\Gamma\, dF \cos\theta}{\pi r^2 v} \tag{1}$$

where r is the distance to the point of emission. We assume that all particle are ionized after travelling a certain distance λ in the plasma. By integration over the surface F, which dimension is larger than the ionization length ($\sqrt{F} \gg \lambda$), the density of the neutral impurities $n(z)$ becomes for $z \le \lambda$

$$n(z) = \int_{\varphi}\int_{r'} \frac{\Gamma \cos\theta}{\pi r^2 v} r'\, d\varphi\, dr' = \frac{\Gamma z}{v\pi}\int_0^{2\pi} d\varphi \int_z^{\lambda} \frac{dr}{r^2}$$

$$= \frac{2\Gamma}{v}\left(1 - \frac{z}{\lambda}\right) \tag{2}$$

with $z = r \cdot \cos\theta$, $r' = \sqrt{r^2 - z^2}$, $dr' = r\,dr/\sqrt{r^2 - z^2}$

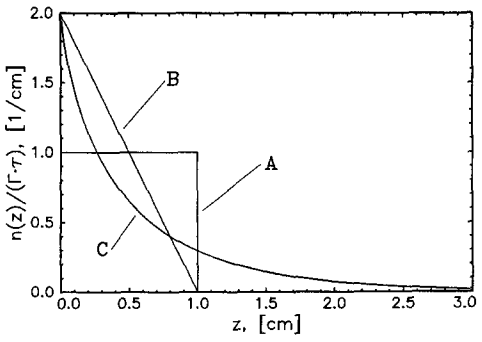

Fig. 1. Normalized density distributions of the neutrals emitted from a infinite extended surface versus the distance from the surface, z (A – for $\theta = 0$ and $\lambda = 1$ cm, B – Eq. (2), C – Eq. (3)).

and thus $r'\,dr' = r\,dr$. Using Eq. (2) the ionization length distribution can be taken into account by the integration:

$$n(z) = \int_z^{\infty} \frac{2\Gamma}{v}\left(1 - \frac{z}{\lambda'}\right)\frac{\exp(-\lambda'/\lambda)}{\lambda} d\lambda'$$

$$= \frac{2\Gamma}{v}\left[\exp\left(-\frac{z}{\lambda}\right) - \frac{z}{\lambda}E_1\left(\frac{z}{\lambda}\right)\right] \tag{3}$$

where $E_1(x) = \int_z^{\infty}(\exp(-t)/t)\,dt$. As a good approximation the following expression can be used [5]: $E_1(x) = [\ln(1 + 1/x) - 0.4/(1 + x)^2]\exp(-x)$. Fig. 1 shows the normalized density distributions for the average value of the ionization length, $\lambda = 1$ cm. Further, the energy of the neutrals E influences via the corresponding ionization length the neutral density distribution. Two main energy distributions for the emitted particles can be distinguished, the Thompson distribution dN^{TH}/dE (characterizing physical sputtering [6]):

$$\frac{dN^{TH}}{dE} = \frac{2UE}{(E+U)^3},$$

$$\frac{dN^{MW}}{dE} = \frac{2}{kT_s}\left(\frac{E}{\pi kT_s}\right)^{1/2} \cdot \exp\left(-\frac{E}{kT_s}\right) \tag{4}$$

with T_s being the surface temperature and the Maxwell distribution dN^{MW}/dE caused by thermal evaporation or thermal desorption. U is the surface binding energy. From Eq. (4) the following expressions can be easily obtained using $\lambda = \tau\sqrt{2E/m}$:

$$\frac{dN^{TH}}{d\lambda} = \frac{8U}{m\tau} \cdot \frac{(\lambda/\tau)^3}{\left[(\lambda/\tau)^2 + 2 \cdot U/m\right]^3} \tag{5}$$

$$\frac{dN^{MW}}{d\lambda} = \frac{4}{\lambda\sqrt{\pi}}\left(\frac{\varepsilon}{kT_s}\right)^{3/2} \cdot \exp\left(-\frac{\varepsilon}{kT_s}\right) \tag{6}$$

with $\varepsilon = m\lambda^2/(2\tau^2)$; τ is the average ionization time and m the mass of the sputtered atoms. Assuming that all particles emitted normally from the surface the effect of the different energy distributions on $n(z)$ can be calculated by

$$n(z) = \int_z^{\infty} \frac{\Gamma}{v} \cdot \frac{dN}{d\lambda} \cdot d\lambda.$$

One obtains for the Thompson distribution:

$$n(z) = \Gamma\left(\frac{1}{2\sqrt{V}}\left[\frac{\pi}{2} - \arctan\left(\frac{\xi}{\sqrt{V}}\right)\right] + \frac{\xi V - \xi^3}{2(\xi^2 + V)^2}\right) \tag{7}$$

and the Maxwell distribution

$$n(z) = \Gamma \cdot \sqrt{\frac{2m}{\pi kT_s}} \cdot \exp\left(-\frac{m}{2kT_s} \cdot \xi^2\right) \tag{8}$$

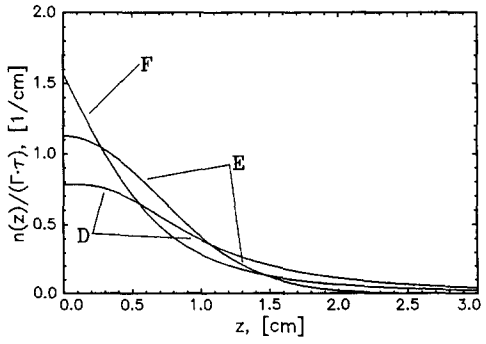

Fig. 2. As in Fig. 1 (D – Eq. (7), E – Eq. (8), F – Eq. (9)).

with $\xi = z/\tau$ and $V = 2 \cdot U/m$. In order to describe the neutral density distribution in the case of physical sputtering Eqs. (3) and (5) should be combined by the integration:

$$n^{\mathrm{TH}}(z) = \frac{8\Gamma V}{\tau} \cdot \int_0^{\infty} \left[\exp\left(-\frac{z}{\lambda}\right) - \frac{z}{\lambda} E_1\left(\frac{z}{\lambda}\right) \right] \times \frac{(\lambda/\tau)^2}{\left[(\lambda/\tau)^2 + V\right]^3} \mathrm{d}\lambda \qquad (9)$$

The analytical distributions for the different cases are presented in the normalized form $n(z)/\int_0^{\infty} n(z)\,\mathrm{d}z = n(z)/(\Gamma \cdot \tau)$ in Fig. 2. A similar integration as in Eq. (9) for the Maxwellian distribution (Eq. (6)) can be carried out. Usefully can be the values for $z = 0$ which do not depend on the plasma parameters:

$$n^{\mathrm{TH}}(0) = \Gamma \sqrt{\frac{m\pi^2}{8U}}, \qquad n^{\mathrm{MW}}(0) = \Gamma \sqrt{\frac{8m}{kT_s\pi}} \qquad (10)$$

It should be noted that the ionization length and the decay length of the neutral density distribution differs significantly in contrast to the often made assumption of their equality.

3. Experimental setup

A 'Li marker' made of an Al–Li alloy (10% Li) with a diameter of 5 mm was embedded in the center of a graphite target (∅30 mm) and was exposed in a steady-state D plasma. The electron density $n = 1 \cdot 10^{11}$ cm^{-3} and temperature $T = 4$ eV have been measured by a reciprocating Langmuir prob. The intensity of the resonance line of Li (671 nm) was measured with an optical multichannel analyzer as a function of distance from the target. Further, the temperature of the surface has been measured. For the above mentioned plasma parameters ionization lengths of about 2 m (for physical sputtering, $E \simeq U/2 = 0.835$ eV) and of about 0.5 m (for thermal sublimation $E \simeq T_s = 0.06$ eV are expected. The ionization rate coefficients of lithium have been taken from [7].

4. Results and discussion

The surface temperature of the target increased owing to the heat load on it during the exposure to the plasma. The intensity of the LiI emission measured 1.3 mm above the target also grew up (see Fig. 3). These dependence indicates that thermal sublimation of the lithium atoms plays a significant role. The target temperature follows the Arrhenius relation with an activation energy of about 0.7 eV. For such an alloy (Al/Li) one would expect a value of about 1.5 eV [8] for the energy of vaporization, which is close to the value for elemental lithium. After exposure the target has been analyzed using XPS (X-ray photoelectron spectroscopy) and AES (Auger electron spectroscopy) techniques and the following composition was found: 5.4% C, 23.7% O, 5.6% Cu, 56.6% Al and 8.7% Li. The surface concentration of lithium strongly influences its erosion yield. In order to obtain the flux of eroded lithium atoms the measured intensity distribution of the line emissions has to compare with the theoretical predictions. We have to calculate a space distribution of the neutrals atoms using Eq. (1) and taking the energy distribution of the emitted neutrals into account. The integration over the circular marker surface with the radius $r_F = 2.5$ mm gives

$$n(z, r_P) = \frac{\Gamma}{\pi} \int_0^{2\pi} \int_0^{r_F} \frac{z r'}{r^3} \mathrm{d}r'\,\mathrm{d}\varphi \int_r^{\infty} \frac{\tau}{\lambda} \frac{\mathrm{d}N}{\mathrm{d}\lambda} \mathrm{d}\lambda \qquad (11)$$

with $r^2 = r'^2 + r_P^2 - 2r'r_P \cos\varphi \cdot \sqrt{1 - (z/r_P)^2}$ and r_P being distance from the centre of the marker spot to the certain spatial point, where the density should be determined. For inner integral in Eq. (11) the analytical Eqs. (7) and (8) can be used. In order to calculate the photon emissivity for the transition from the level k to level i, which is really measured in the experiment, we have to know the density of the excited neutral atoms of level n_k. For the one dimensional case (only motion in direction of z is considered and the neutrals, which are in the ground

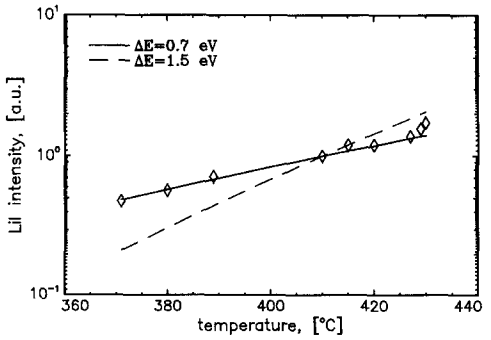

Fig. 3. Measured LiI (671 nm) intensity at a distance of 1.3 mm from the marker spot normalized to the value at $T_s = 410$°C (symbols) together with the dependencies for two activation energies ΔE (lines).

state, leave the surface with the same velocity v) it can be easily shown that

$$n_k(z) = \frac{\Gamma n_e X_{gk}}{v(\Sigma_{i\le k} A_{ki} - v/\lambda)} \times \left[\exp\left(-\frac{z}{\lambda}\right) - \exp\left(-\frac{\Sigma_{i\le k} A_{ki}}{v} z\right)\right] \quad (12)$$

with the maximum at $z_{max} = \ln(\lambda \cdot \Sigma_{i\le k} A_{ki}/v)/(A/v - 1/\lambda)$; λ is the average ionization length, X_{gk} is the rate coefficient for the excitation of level k from the ground state ($T_e = 4$ eV, $X = 5 \cdot 10^{-7}$ cm^3 s^{-1}), $\Sigma_{i\le k} A_{ki}$ is the spontaneous transition probability from level k into all lower states i. The main parameter is $\zeta = \lambda \cdot \Sigma_{i\le k} A_{ki}/v$ which is for our conditions much greater one ($\zeta \simeq 15000$), therefore the so-called corona population equilibrium approximation can be used and we obtain finally for the photon production in a certain line-of-sight volume at the distance from the target z:

$$P(z) = \frac{\pi d_s^2}{4} \int_{-d_p/2}^{d_p/2} XBn_e n(z, r_p)\,dx \text{ (photons/s)} \quad (13)$$

where the B denotes the branching ratio $B = A_{ki}/\Sigma_{i\le k} A_{ki}$ ($B = 1$ for LiI 671 nm), $d_s = 0.7$ mm is the diameter of the line-of-sight, $d_p = 30$ mm is the diameter of the plasma column and $r_p = \sqrt{z^2 + x^2}$. Fig. 4 shows calculated results using Eq. (13) for both thermal sublimation (Eq. (8)) and physical sputtering (Eq. (7)). The decay lengths of the measured and also of the calculated distributions strongly differs from the ionization lengths. This is owing to the point-like source, which emits the atoms in all directions of the half-sphere with nearly the same probability. In order to get a satisfactory agreement with the experimental results a value of about $\Gamma = 2.5 \cdot 10^{13}$ cm^{-2} s^{-1} for the flux of eroded lithium atoms has been taken in the calculations both for physical sputtering, $\Gamma_{phys} = \Gamma$, and thermal sublimation, $\Gamma_{subl} = \Gamma$ (Fig. 4). For physical sputtering one gets $\Gamma = \Gamma_D \cdot Y = n_e c_s \cdot Y \simeq 1.4 \cdot 10^{17} \cdot Y$ (cm^{-2} s^{-1}) with c_s being the sound speed. The sputtering yield, Y, of elemental lithium by deuterium equals ≈ 0.006 [9]. Taking in a first approximation the low surface concentration of lithium (as measured by the surface analysis techniques) into account one should take a much lower sputtering yield of about $Y \simeq 0.006 \cdot 0.087$, which results in $\Gamma_{phys} = 7.3 \cdot 10^{13}$ cm^{-2} s^{-1}. As seen in Fig. 4, physical sputtering only slightly influences the shape and the magnitude of the density distribution owing to the much larger ionization lengths (see Fig. 4). For thermal sublimation one would expected $\Gamma_{subl} = 2 \cdot 10^{14}$ cm^{-2} s^{-1} at the target temperature $T_s = 410$°C [8]. This value is much larger than the measured one. But in [8] the alloy surface was predominantly covered by a complete lithium overlayer as a result of combined segregation and diffusion. This is certainly not true in our experiment (see the surface composition given before).

It should be noted that this particular example shows predominantly geometrical effects, because only few Li atoms are ionized in the regions that is spectroscopically observed. In cases with much stronger ionization information about electron density or temperature, for example, can be inferred.

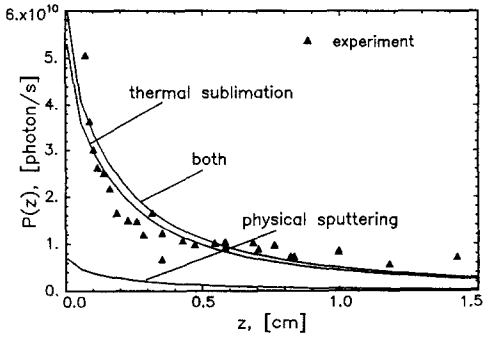

Fig. 4. LiI intensity versus distance from the marker spot in comparison with the calculated curves using Eqs. (11) and (13) for both physical sputtering and thermal sublimation (at $T_s = 410$°C).

5. Summary

Analytic formulae are given for the density distributions of neutrals emitted from surfaces. These expressions can be used, as shown experimentally in the PSI-1 plasma generator, for determination of the flux of the emitted particles. If this value is known (from non-spectroscopic information), excitation rate coefficients or plasma parameters can be obtained. Further, numerical calculations with Monte-Carlo transport codes such as the WBC [10], the DIVIMP [11] and the ERO codes [12] can be validated using the derived expressions. For example, time and space intervals can be optimized.

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