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# Modelling of charged particle dynamics in the sheath and plasma-facing surface sputtering

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#### Abstract

In this work a useful analytical approximation for the electric potential profile in the presence of an oblique magnetic field is suggested. It describes the potential profile dependence on the magnitude and angle of a magnetic field and plasma parameters in the Debye sheath and the magnetic pre-sheath. It is in good agreement with the Chodura and Stangeby solutions and respective PIC simulations performed with the SPICE2 code. The influence of the magnetic field inclination angle on the angle and energy distributions of ions which reach the wall, and thus on the effective sputtering, is analyzed for various first wall materials.

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## 1. Introduction

For a successful realization of the ITER project it is very important to study the plasma-surface interaction processes. Many properties of the core plasma such as plasma confinement time, plasma content and temperature are controlled by these processes. It is necessary to correctly determine the inflow and outflow of charged particles at material surfaces in order to determine hydrogen isotope implantation and reflection, plasma–facing material

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sputtering and secondary emission, and to analyze experimental data in the plasma sheath. The angle and energy of the plasma species impinging on the surface of fusion devices have a strong influence on the physical sputtering and reflection. They are, however, strongly determined by the local electric and magnetic fields in front of the surfaces. It has been shown that the increasing of the magnetic field inclination angle produces a negligible change in the value of the floating potential, but the potential redistributes so that both the potential drop in the magnetic presheath and the length of the magnetic pre-sheath increase [Chodura (1982)]. The calculation of the electric field potential distribution in the presence of an inclined magnetic field in the Debye sheath and the magnetic pre-sheath is rather complicated computational task. In this work a useful analytical approximation for the electric potential profile is suggested, which is simpler than the integral equations in [Chodura (1982), Stangeby (2012)]. Using suggested solutions the influence of the magnetic field inclination angle on the angle and energy distributions of D<sup>+</sup> and Be<sup>4+</sup> ions which reach the wall, and thus on the effective sputtering, is analyzed for various first wall materials. The influence of the plasma temperature and the magnetic field strength on the plasma-facing components' sputtering was investigated.

## 2. An analytical model for the electric field in the presence of an oblique magnetic field

The plasma potential can be calculated using the Poisson equation as in [Chodura (1982), Stangeby (2012)]:

$$\frac{d^2\varphi}{dx^2} = 4\pi e(N_e - N_i) \tag{1}$$

where  $N_{ei}$  are the electron and ion densities, respectively and e is the absolute value of the electron charge. The equation (1) has a dimensionless form:

$$\frac{d^2\Psi}{d\xi^2} = (n_e - n_i) \tag{2}$$

where  $\psi = e(\varphi - \varphi_0)/kT_e$  represents the normalized potential,  $\varphi_0$  is the potential at the sheath/presheath boundary,  $n_{e,i} = N_{e,i}/N_0$  - the electron and ion densities normalized by the plasma density,  $\xi = x/r_d$  is the distance from the surface in units of the Debye length.

We assume the Boltzmann distribution for the electron density:  $n_e = \exp(\psi)$ .

The ion density in contrast to the electron one is derived from the conservation of the ion flux. In the Debye sheath the ion flux velocity increment corresponds to the potential drop. However, in the magnetic pre-sheath due to the ion gyro motion this relation is more complex: the ion flux velocity decreases and the ion density approaches to the electron density. In the MHD theory the magnetic pre-sheath is considered as quasineutral. But on account of the presence of the electric field in the magnetic pre-sheath we assume that the ion and electron density difference corresponded to the electric field potential occurs there, though it is rather small.

So, for a potential profile description in the magnetic pre-sheath we have made two assumptions. Firstly, as the magnetic pre-sheath is quasineutral, the ion and electron density difference related to the electric field potential is small. This allows us to assume a linear dependence of the potential on the density difference as a first order approximation:

$$\Psi \approx \frac{\Psi_{mps}}{\Delta n_{mps}} (n_i - n_e) \tag{3}$$

where  $\Delta n_{mps}$  is the ion and electron density difference at the magnetic pre-sheath - the Debye sheath boundary where  $\Psi = \Psi_{mps}$ ,  $\Psi_{mps} = \ln(\cos \alpha)$  is the normalized potential drop in the magnetic pre-sheath as derived in [Stangeby (2012)],  $\alpha$  is an angle between the magnetic field and the surface normal.

Secondly, we assume the electric field is equal to the value of the average electric field in the magnetic presheath at  $\Psi = \Psi_{mps}/2$ :

$$\frac{d\Psi}{d\xi} \Big|_{\frac{\Psi_{mps}}{2}} = \frac{\Psi_{mps}}{L_{mps}} \tag{4}$$

where  $L_{mps} = 2 \cdot \rho_{iCs}/r_d \cdot \sin \alpha$  is the magnetic pre-sheath length,  $\rho_{iCs}$  is the Larmour radius for the ion acoustic velocity.

Solving the Poisson equation  $\Delta \psi = n_e - n_i$  and taking into account that the potential drop  $\lambda$  and the electric field in plasma are zero we obtain the following dimensionless approximation for the potential distribution in the magnetic pre-sheath:

$$\lambda = \lambda_{mps} \cdot \exp(-\sqrt{-\frac{\Delta n_{mps}}{\lambda_{mps}}} (\xi - \xi_{mps}))$$
 (5)

where  $\Delta n_{mps} = -\ln(\cos\alpha)((\rho_{iCs} / r_d)\sin\alpha)^{-2}$  and  $\xi_{mps}$  is the magnetic pre-sheath/the Debye sheath boundary. In the Debye sheath the solution of the Poisson's equation was found as following:

$$\lambda(\xi) = \lambda_w + Q - Q \exp(-a\xi) \tag{6}$$

where  $\lambda_w$  is the value of the floating potential and parameters a and Q depend on plasma parameters, magnetic field strength and angle:

$$\lambda_w = \frac{e(\varphi_w - \varphi_0)}{kT_e} = \frac{1}{2} \ln \left( 2\pi \frac{m_e}{M_i} \frac{T_e + T_i}{T_e} \right) \tag{7}$$

$$a = \frac{\sqrt{-\Delta n_{mps} \lambda_{mps}} - \sqrt{2 \exp(\lambda_w) + 4 \cdot \cos \alpha \sqrt{1 - (\lambda_w - \lambda_{mps})} + C_1}}{\lambda_w - \lambda_{mps}}$$

$$Q = \frac{1}{a} \cdot \sqrt{2 \exp(\lambda_w) + 4 \cos \alpha \sqrt{1 - (\lambda_w - \lambda_{mps})} + C_1}}$$

$$C_1 = -\Delta n_{mps} \lambda_{mps} - 6 \cos \alpha$$
(8)

The coordinate  $\xi_{mps}$  of the magnetic presheath/the Debye sheath boundary was obtained from (4):

$$\xi_{mps} = -\frac{1}{a} \ln(\frac{\lambda_w - \lambda_{mps} + Q}{O}) \tag{9}$$

Fig. 1a demonstrates good agreement of the potential profiles calculated using the approximated potential model (5) and (6), the Chodura and Stangeby solutions [Chodura (1982), Stangeby (2012)] and respective particle-in-cell (PIC) simulations performed with the SPICE2 code (Dejarnac et al. (2008)). ( $T_e = T_i = 30 \text{ eV}$ , B = 3T,  $n=10^{14} \text{ cm}^{-3}$ ,  $\alpha = 80^\circ$ ). The confirmation of our assumption (3) in the magnetic pre-sheath is presented in Figure 1b. Thus, the suggested expressions for the electric potential distribution in the Debye sheath (6-8) and magnetic pre-sheath (5) can be successfully used instead of the numerical solution of the Poisson equation in the modeling of the plasma surface interaction processes.

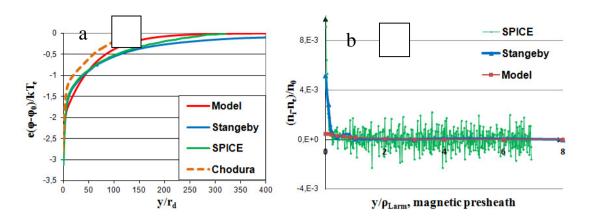


Fig. 1. a) The potential profiles obtained from the model (5-6), [Chodura (1982), Stangeby (2012)] and code SPICE2 [Dejarnac et al. (2008)]  $(T_e = T_i = 30 \text{eV}, n = 10^{14} \text{cm}^3, B = 3.2 \text{ T}, \alpha = 80^\circ)$ . b) The ion and electron density difference in the magnetic pre-sheath obtained from the model (3) and (Stangeby (2012))  $(T_e = T_i = 30 \text{ pB}, n = 10^{14} \text{ cm}^3, B = 3.2 \text{ T}, \alpha = 80^\circ)$ .

# 3. Dependence of the sputtering yield on the magnetic field inclination angle

For particle tracing modeling the equations of motion in electric and magnetic fields are numerically solved. The simulated plasma-wall transition layer includes the Debye sheath and the magnetic pre-sheath. The simulated system is bounded by the bulk equilibrium deuterium plasma containing electrons and ions with the constant densities  $n_e = n_i$  and the temperatures  $T_e = T_i$ . The D<sup>+</sup> and Be<sup>4+</sup> ions were injected from the  $10\rho_{iCs}$  with the shifted Maxwell velocity distribution. The magnetic field is uniform with a certain inclination  $\alpha$ . The electric field is calculated from the suggested model for the deuterium plasma (5-8). The magnetic field angle influence on the energy and angular distribution of impinging on the surface ions was investigated. The calculations were carried out for 100000 ions for each angle of the magnetic field. It was found that the average incident angle (measured from the surface normal) increases with the magnetic field inclination angle. The angular distributions obtained from the model show good agreement with the respective simulations performed by the SPICE2 code and taken from [Kawamura et al. (2009)] (Figure 2a). The influence of the plasma temperature and magnetic field strength on the angular distribution of ions impinging the plasma-facing surfaces was investigated. However, it was found that these effects are negligible.

Using the obtained angular and energy distributions the dependence of the sputtering coefficient on the magnetic field inclination angle was calculated with the Eckstein formula [Behrisch et al. (2007)] (figure 2b). The calculations were carried out for incident  $D^+$  and  $Be^{4+}$  ions on the Be and C surfaces. One can see that the sputtering coefficient by  $D^+$  ions gradually grows with increasing of the magnetic field angle from  $0^{\circ}$  to  $60^{\circ}$ , but further, from  $60^{\circ}$  to  $80^{\circ}$ , the coefficient increases almost twice. However, the self-sputtering coefficient by  $Be^{4+}$  ions has already increased twice up to  $60^{\circ}$  of the inclination magnetic field angle and further grows 3 times more. The plasma temperature effects on the sputtering coefficient in the following way: the sputtering does not substantially depend on the magnetic field angle at the low plasma temperature ( $\sim$ 10 eV); however, the temperature increasing leads to the significant growth in the magnetic field inclination angle.

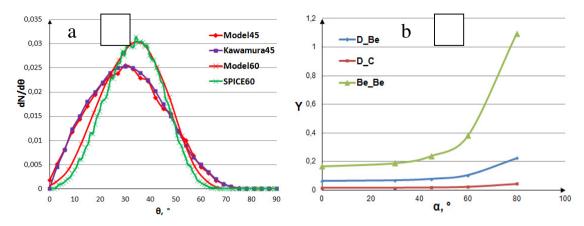


Fig. 2. a. The angular distributions calculated from the model and SPICE2 code ( $T_e = T_i = 30 \text{eV}$ ,  $n = 10^{14} \text{cm}^{-3}$ , B = 3T) for  $\alpha = 60^\circ$ ; from the model and PIC-code [Behrisch et al. (2007)] ( $T_e = T_i = 30 \text{eV}$ ,  $n = 10^{12} \text{cm}^{-3}$ , B = 5 T) for  $\alpha = 45^\circ$ . b. The magnetic field angle influence on the Be and C sputtering yield by incident D<sup>+</sup> and Be<sup>++</sup> ions ( $T_e = T_i = 20 \text{eV}$ ,  $n = 3 \times 10^{12} \text{cm}^{-3}$ , B = 4.1 T).

#### 4. Conclusion

In this work a useful analytical approximation for the electric potential profile in the presence of an oblique magnetic field is suggested. This expression describes the potential profile dependence on magnitude, angle of magnetic field and plasma parameters in the Debye sheath and the magnetic pre-sheath. It is in good agreement with the Chodura and Stangeby solutions and respective PIC simulations performed with the SPICE2 code.

The energy and angular distributions of particles reaching the wall at different angles of the magnetic field inclination were calculated. It was obtained, that average ion incident angle increases with the magnetic field inclination angle more than 60°. The angular distributions obtained using the suggested model show good agreement with the respective simulations performed by SPICE2 code and taken from [Kawamura et al. (2009)]. It is found that the plasma temperature and the magnetic field strength practically do not affect the most probable incident ion angle.

Using these results the sputtering coefficient dependence on the magnetic field angle for different materials of the first wall was calculated. Also the self-sputtering of Be was considered. It was shown that the sputtering yields considerably increase at magnetic field inclination angles more than 60°. Thus the regions of the first wall on which the magnetic field comes under strong sliding angles are critical in terms of sputtering increase.

The obtained results can be used to construct the closed model of ion and electron recycling in the sheath of a fusion reactor.

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