Predicting Wall Conditioning

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Theory

When a material has been subjected to impurities, these impurities will be stored in interstitial lattice sites (LS). The base material atoms are bound by a certain energy E_b whilst the trapped impurity is bound by E_t, as most often $\mid E_t \mid < \mid E_b \mid$, wall conditioning in fusion reactors is effective. In general GDC (glow discharge wall conditioning) creates low energy ions which propagate to the wall as no magnetic field is present. Ion cyclotron wall conditioning creates low-energy charge exchange neutrals (i.e neutrals who have gained their energy through charge exchange) who, as they are not confined, move towards the wall. Ideally these ions and neutrals have energies sufficient to de-trap (sputter) the impurities but are still below the energy necessary to sputter the base material. Mathematically we can express the amount of impurities leaving the wall per area (m^2) as a functional of the form:

$$\mathcal{I}[n] = \sum_j \int_E \int_\theta Y_{jI}(n(t,\mathbf{r}),E,\theta)\mathfrak{F}_j(E,\theta) \tag{1}$$

Whereby $Y_{Ij}(n(t,\mathbf{r}),E,\theta)$ is the impurity concentration-, energy- and angle of incidence-dependent impurity sputtering rate (i.e #out/#in) for incoming species j and $\mathfrak{F}_j(E,\theta)$ is the incoming particle distribution ($\frac{\text{particles}}{m^2 s}$) for species j. The base material sputtering rate may be given by:

$$B = \sum_j \int_\theta \int_E Y_{jB}(E,\theta)\mathfrak{F}_j(E,\theta) \tag{2}$$

In full, the total amount of particles leaving the wall per second per unit area is thus:

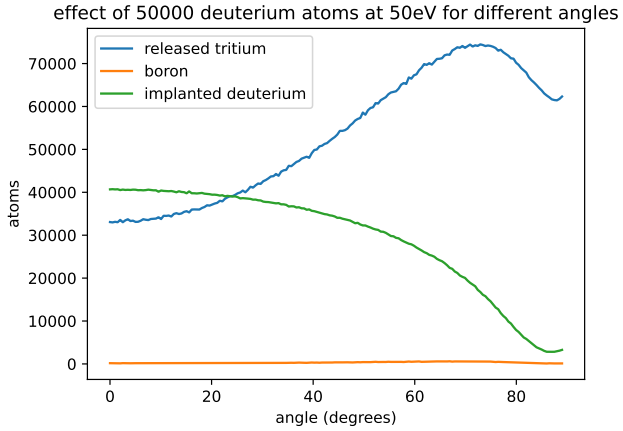
$$W(t) \triangleq \mathcal{I}[n] + B = \sum_j \int_\theta \int_E \left\{Y_{jI}(n(t,\mathbf{r}),E,\theta) + Y_{jB}(E,\theta)\right\}\mathfrak{F}_j(E,\theta) \tag{3}$$

Simulation: homogeneous doping and erosion

To simulate Y_{jI} it is necessary to create a model, the chosen model is 1D and consists of a slab of the base material with a certain concentration of E_t bound impurities. As we will be using the BCA, more specifically rustBCA[1], our simulations are dependent on how we choose our parameters, namely the cutoff energy E_c, the displacement energy E_d , the bulk binding energy E_b and the surface binding energy E_s [2]. As we're dealing with sputtering, we will ignore E_d and take E_c to be small enough (e.g 1% of the input energy). In most codes E_b is taken to be 0 and only E_s is varied, we will not proceed this way as this omits some physics, we will take E_b to be a reported value for the base material and $E_s = \Delta H_s - E_b$, i.e the heat sublimation is the energy to dislodge an atom from the lattice and transport it to outside the material. As a lot of current research on wall conditioning concerns boron on tungsten or graphite substrates, with boron having a measured density of 1.1 g/cm^3 on TOMAS, we will focus on boron of number density

$$\frac{1.1}{10.81} \times \frac{N_a}{10^{24}} = 0.06128 \frac{\text{atoms}}{\text{Å}^3} \tag{4}$$

Note that 1.1 g/cm^3 is considerable lower than in most of the literature, we assume that this is inherent to the method of layer growth used, namely magnetron sputtering. For pure boron $\Delta H_s = 5.6$eV [5] and as usually $E_s = 5.73$ is taken, we will take $E_b = 0.13$eV. For the impurities we will assume they have both E_s and E_b equal zero. The simplest model considers the impurities to be homogeneously distributed in the slab and to erode homogeneously. Simple BCA simulations using these parameters for different angles shows the following behaviour (20% impurity doping):



Although this yields insight in how angle dependence plays a role, it is not in general easily measurable. A quantity that is in general measured is the outgassing

in function of time, as such we need to add time-dependence to our model. The amount of impurities in a slab of area A and depth D prior to any wall conditioning may be given by $N_0 = n_0 \times A \times D$, after one timestep Δt the amount will have been reduced by $\sum_j Y_{jI}(n(t), E, \theta)\mathfrak{F}_j(E, \theta) \times A \times \Delta t \triangleq \mathcal{I}[n(t)]A\Delta t$. The amount of impurities in the material thus follows (if we assume homogeneous erosion):

$$\frac{\mathrm{d}N(t)}{\mathrm{d}t} = AD\frac{\mathrm{d}n(t)}{\mathrm{d}t} = -A\mathcal{I}[n(t)] \tag{5}$$

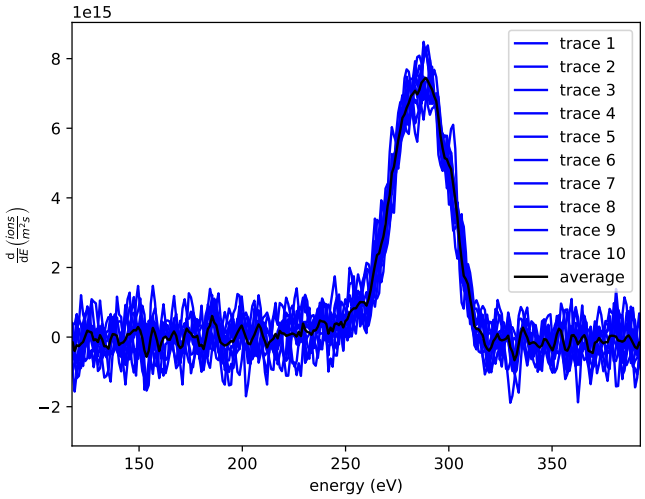
We thus have that the concentration of impurities in the slab changes as

$$\frac{\mathrm{d}n}{\mathrm{d}t} = -\frac{\bar{\mathcal{I}}[n(t)]}{D} \tag{6}$$

We need to solve this equation to determine the amount of impurities sputtered per second per unit area $\bar{\mathcal{I}}[n(t)]$, e.g forward euler we would start from a certain $n = n_0$ and change n according to

$$\Delta n = -\frac{\bar{\mathcal{I}}[n(t)]}{D}\Delta t \tag{7}$$

We will start with GD in H_2 of which we have ion energy distributions from an RFEA:



Here obviously $\bar{\mathfrak{F}}_j(E, \theta) \triangleq \frac{\mathfrak{F}_j(E,\theta)}{\Delta E}$ is the y-axis, we also assume equal angle likeliness, as such:

$$\mathcal{I}[n] = \frac{1}{N}\sum_j \sum_E \sum_\theta^N Y_{jI}(n(t, \mathbf{r}), E, \theta)\bar{\mathfrak{F}}_j(E, \theta)\Delta E \tag{8}$$

Where we kept the summation over j as multiple species may be present which may be accounted for (not only H^+ but also H_2^+, H, H_3^+,...)

Compare with experiments

$\mathfrak{F}_j(E) \triangleq \int_\theta \mathfrak{F}_j(E,\theta)$ is a measureable quantity, for example on TOMAS the neutral fluxes are measureable [4] as well as the ions [3]. As such, an angle distribution needs to be chosen, e.g

$$\tilde{\mathfrak{F}}_j(E,\theta) \triangleq \frac{2cos^2(\theta)}{\pi}\mathfrak{F}_j(E) \tag{9}$$

Y_{jB} on it's own is straightforward to simulate using e.g rustBCA using known material parameters, the difficulty lies in simulating the compound, and thus devising Y_{jI}.

References

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[3] A. Goriaev, K. Crombé, D. López-Rodríguez, S. Möller, J. Buermans, M. Verstraeten, D. Castaño Bradwil, L. Dittrich, P. Petersson, and Yu. Kovtun. First studies of local ion fluxes in radio frequency plasmas for ion cyclotron wall conditioning applications in the tomas device. *AIP Conference Proceedings*, 2984(1):040007, 08 2023.

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[5] E. Vietzke, V. Philipps, and K. Flaskamp. High temperature erosion of boron/carbon materials. *Journal of Nuclear Materials*, 196-198:1112–1117, 1992. Plasma-Surface Interactions in Controlled Fusion Devices.