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 $E_t > E_b$, wall conditioning in fusion reactors is effective. In general 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 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:

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

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. A simple first step would be to consider the impurities to be homogeneously distributed in the slab and to erode homogeneously. 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 $\sum_j Y_{jI}(n(t), E, \theta)\mathfrak{F}_j(E, \theta) \times A \times \Delta t \triangleq \mathcal{I}[n(t)]A\Delta t$ whereby $\mathfrak{F}_j(E, \theta)$ is the amount of particles of species j per unit area per second. The amount of impurities in the material thus follows (if we assume homogeneous erosion):

$$\frac{\mathrm{d}N(t)}{\mathrm{d}t} = AD\frac{\mathrm{d}n(t)}{\mathrm{d}t} = -A\mathcal{I}[n(t)] \tag{4}$$

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

$$\frac{\mathrm{d}n}{\mathrm{d}t} = -\frac{\bar{\mathcal{I}}[n(t)]}{D} \tag{5}$$

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

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

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 [2] as well as the ions [1]. As such, an angle distribution needs to be chosen, e.g

$$\tilde{\mathfrak{F}}_j(E, \theta) \triangleq \frac{2cos^2(\theta)}{\pi}\mathfrak{F}_j(E) \tag{7}$$

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

[1] 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.

[2] D. López-Rodríguez, K. Crombé, A. Goriaev, J. Buermans, A. Adriaens, Yu. Kovtun, L. Dittrich, P. Petersson, T. Wauters, and S. Brezinsek. Characterization of plasma parameters and neutral particles in microwave and radio frequency discharges in the toroidal magnetized system. *Review of Scientific Instruments*, 95(8):083542, 08 2024.