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, go towards the wall. Ideally these neutrals have energies sufficient to de-trap (sputter) the impurities but low enough energies to leave the base material intact. Mathematically we can express the amount of impurities leaving the wall as:

$$I(t) = \sum_j \int_E Y_{jI}(E,t)\mathfrak{F}_j(E) \tag{1}$$

Whereby $Y_{Ij}(E,t)$ is the energy and time-dependent impurity sputtering rate (this is time-dependent as the impurity concentration will decrease over time) for incoming species j and $\mathfrak{F}_j(E)$ is the incoming particle distribution (particles/s) for species j. The base material sputtering rate may be given by:

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

Where in the base material sputtering rate may be assumed to not be time-dependent as the material is homogeneous. In full the total amount of particles leaving the wall per second is thus:

$$W(t) \triangleq I(t) + B = \sum_j \int_E \{Y_{jI}(E,t) + Y_{jB}(E)\}\,\mathfrak{F}_j(E) \tag{3}$$

$\mathfrak{F}_j(E)$ is a measureable quantity, for example on TOMAS the neutral fluxes are measureable [2] as well as the ions [1]. Y_{jB} Is straightforward to simulate using e.g rustBCA using known material parameters, the difficulty lies in simulating Y_{jI}.

Simulation input

To simulate Y_{jI} it is necessary to create a model, this model 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.

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.