Effect of reactor-relevant parameters on Be sputtering

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ITER aims to be the first fusion reactor reaching ignition, based on a deuterium (D)-tritium (T) plasma. Its success highly depends on understanding the interplay between the plasma particles and the wall components. Due to its design, the conditions (e.g. temperature, particle flux and thermal loads), and thus the requirements for the wall material, vary with location in the reactor. The main wall of ITER will be made of beryllium (Be). Therefore, quantifying the Be erosion as well as identifying the sputtered species and understanding the underlying mechanisms is essential, not only from the wall life-time point of view, but also in order to reliably explain the impurity transport, re-deposition and re-erosion patterns.

The experimental work on Be exposed to D plasmas is extensive. Most studies have been performed in linear devices where it is possible to control the exposure (plasma and substrate) conditions. The experiments provide a broad database for the erosion yields, but an incomplete description of the mechanisms.

On the other hand, these atomic-scale dynamics in materials can be studied using Molecular Dynamics (MD) simulations, which include many-body effects, such as chemical erosion and molecule formation. Therefore, we present a MD study on the Be erosion under fusion relevant conditions, scanning over the plasma parameters and surface conditions, and focusing on the chemical effects. To this end, we simulated D irradiation of Be surfaces, varying the D impacting energy ($3 - 100$ eV), angle ($0 - 70^\circ$) and flux ($10^{27} - 10^{28}$ m^{-2}s^{-1}), as well as surface temperature ($200 - 1440$ K) and D concentration ($0 - 50\%$).

Our results show that the Be erosion peaks at impacting energies of 50 eV, due to the swift chemical sputtering mechanism. These erosion yields are suppressed when increasing the D concentration in the surface, due to the dilution of the Be surface atoms. Furthermore, the BeD sputtering does not depend as strongly on the incoming ion angle as the total Be sputtering. These results show little dependence on the D flux $-$ within the range studied here $-$, but strongly on the substrate temperature. The Be erosion ramps up at temperatures above 600 K, as the D desorbs instead of piling up at the surface as at lower temperatures. A wide range of different molecules are sputtered, mainly BeD or BeD_2, but some larger ones (BeD_4, Be_2D_2, Be_3D_5, etc.) are also observed.