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Computational analysis of physical and chemically assisted physical sputtering in plasma-facing components

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Understanding plasma-wall interactions is crucial in the development of fusion reactors. These interactions could cause performance loss and contribute to tritium retention by eroding plasma-facing components (PFCs) through physical or chemically assisted physical sputtering (CAPS) [1]. This makes the investigation of sputtering pivotal in fusion reactors. Specifically, CAPS, and more generally the behavior of molecules released from PFCs, where a data gap is evident.

To address this gap, our study focuses on beryllium (Be), for which a large body of experimental data has been obtained from JET, and where the presence of CAPS is confirmed [2, 3]. Since there is a correlation between CAPS and plasma particle content in the surface, we investigate the erosion of Be structures with different surface concentrations (obtained by kinetic Monte Carlo technique [4]).

The Sputtering is modeled by molecular dynamics (MD) simulations, with an extra focus on CAPS. Additionally, binary collision approximation (BCA) calculations are performed for comparison, since BCA increases computational efficiency by neglecting many-body interactions. However, this superior efficiency is accompanied by lower accuracy.

We find that the balance between physical sputtering and CAPS is clearly impacted by changes in the plasma particles'properties, including isotope type, impact energy, and incident angle. Moreover, we evaluate the effect of the plasma particle concentration in the surface layers, on the contribution of CAPS to the total sputtering yield and on the types of sputtered molecules. Finally, we compare the results of BCA and MD simulations to determine if and where BCA calculations are valid.

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