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Computer study of sputtering mechanisms of fusion relevant materials

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Sputtering of the wall materials of fusion reactors will both affect the plasma as well as the longevity of the wall itself. Even though sputtering as a phenomenon has been known for a long time, the intricate details are still not fully understood. Especially if the wall material is not a pure metal, but either an alloy or decorated by some other elements, the sputtering becomes more complex. At high energy the sputtering yield is dominated by the deposited energy in the surface region, and channeling is, therefore, affecting the sputtering and reflection dramatically. However, at lower energies, the mechanisms are different, as it gets more dependent on the exact configuration of surface atoms and impurities on the surface. We study, utilizing Molecular Dynamics simulations, the atomistic phenomenon of sputtering at low energies (up to around 1 keV). The table data gathered is sputtering and reflection yields, and outgoing angle and energy distributions. In addition to this data needed as input in larger scale models, we can also identify the exact mechanisms present during the sputtering event and identify them for different surface orientations. These mechanisms become even more complex when the surfaces are not pure, for instance decorated with deuterium, which is fusion relevant. We identified that deuterium decoration of the surface will affect the sputtering yield of the tungsten surface.

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