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Present status of modelling dynamically modifying rough and/or crystalline surfaces under energetic particle bombardment: Consequences for reflection and sputter yield distributions

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Key input quantities for the modelling of plasma-wall interactions are the energy and angular distributions of the particles impinging onto the wall as well as the corresponding distributions for the particles (re-)entering the plasma.
Traditionally the focus has been on the modifications of the wall induced by the incoming particle influx (i.e. sputtering) and extensive simulation efforts have provided a good understanding of the processes involved (preferential sputtering, recoil implantation etc.) and the main consequences of surface roughness, which typically reduces the effective sputter yield. Significantly less effort has been dedicated to the analysis of the effects of the resulting morphology changes on the distributions of reflected particles. Here we show that - in contrast to the case of sputter yields - changes of the reflected particle distributions are not only quantitative but also qualitative, ie. specular reflection is often strongly suppressed and the preferred direction of reflection is sometimes - and perhaps surprisingly - even shifting towards(!) the impact direction for non-perpendicular influx. BCA-based simulations for a number of cases relevant for fusion applications (e.g. Hydrogen on tungsten and on FeW-systems) using SDTrimSP-2D and molecular dynamics (MD) simulations are given and the involved mechanisms are clarified. As consequence an efficient representation of the reflection distributions is required. For the parametrization in terms of angles and energies an approach resting on a hemispherical orthogonal function system with Chebyshev-based regression coefficients appears beneficial in terms of storage and access efficiency. Consequences for PWI-experiments and simulations will be discussed.

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