Atomistic modeling of plasma-wall interactions using machine learned potential energy functions

L. Chen, A. Kaiser, M. Probst
University of Innsbruck, Institute of Ion Physics and Applied Physics, 6020 Innsbruck, Austria
lei.chen@uibk.ac.at

We show that the sputtering from a beryllium surface by Be or D impacts can be modelled by molecular dynamics simulations using neural network trained potentials. Its accuracy rivals often computationally infeasible direct ab initio molecular dynamics and exceeds the quality of other approaches while allowing system sizes and simulation times similar to those accessible by conventional force fields.

The Be self-sputtering yield obtained for incident energies below 100 eV agrees perfectly with results from ab initio molecular dynamics simulations and compares well with earlier calculations with pair potentials and bond-order potentials (Figure 1) [1].

The sputtering yield from a Be(0001) surface obtained by impact of D atoms with 100 eV kinetic energy obtained by the same method is 2%, which coincides with data from Björkas et al. [2]. Additionally, retention and reflection rates of D on Be surface have been evaluated. Presently we are developing neural network potentials for the ternary H/Be/W system.

Figure 1. Dependence of the self-sputtering yield for the Be(0001) surface on the incident energy. NNP is the acronym of neural network potential.


This work has partially been carried out within the framework of the EUROfusion Consortium. We have received funding from the Euratom research and training programme 2014-2018 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.