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# Machine learning plasma-surface interface for sputtering simulations

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A computational plasma-surface model of sputtering and deposition requires a consistent coupling of the surface dynamics and the plasma transport phenomena. The respective length and time scales of both, the solid and the plasma, span orders of magnitude, rendering a consistent coupling difficult. We investigated the applicability of a machine learning (ML) surrogate model for bridging the inherent scales with a high physics-fidelity regression model at moderate computational cost. The proof of principle is proposed for sputtered particle energy-angular distributions, obtained for different input energy distributions of Ar ions impinging a Ti-Al composite using atomistic Monte Carlo surface simulations.

This work initially collects the findings previously proposed in [1]. Specifically, a multilayer feedforward neural network was trained and verified with a set of incident/outgoing distributions. An error analysis is carried out for the obtained training results, assessing their quality and validity for different sets of hyperparameters. The aspect of generalization of the trained networks for the prediction of sputtered particle energy-angular distributions for unknown, arbitrarily shaped incident ion energy distributions is demonstrated. The present contribution subsequently elaborates on two related aspects pursued within the context of a ML plasma-surface interface model:

(1) The unsupervised analysis of an extended set of particle distributions based on convolutional autoencoders. Therefor, a significantly reduced latent parameter space is found to be sufficient to parameterize the distributions for Ar ions sputtering a binary Ti-Al composite with different chemical compositions. (2) The methodology is transferred to a sparse data set including the surface state from reactive molecular dynamics simulations of Ar ions and Al neutral particles incident on an Al surface for energies typical for deposition (~ eV) and up to typical sputtering energies (> 100 eV).

For both aspects a reliable and data-compact scale bridging is discussed. These models will hence prepare the path for a comprising ML plasma-surface model. The conceptual methodology is envisioned also for cases with more complex surface and gas compositions, e.g., reactive sputtering or reactive ion etching.

[1] F. Krüger, T. Gergs, and J. Trieschmann, Plasma Sources Science and Technology 28, 035002 (2019)