Coupling sputtering and transport simulations through a machine learning plasma-surface interface

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Thin film processing by means of plasma sputter deposition inherently depends on the interaction of energetic particles with a target surface and the subsequent transport of film forming species through the plasma. The length and time scales of the underlying physical phenomena of both the solid and the gas phase span orders of magnitude. Advantage can be taken of these well separated scales by modeling the solid and the gas phase independently. A unified model then requires bridging of the respective models and scales. Surface properties may be calculated from a surface model and stored for a number of representative incident particle energy distribution functions. For this purpose, dynamic transport of ions in matter based TRIDYN [1] simulations are used to calculate sputtered particle distributions for Ar projectiles bombarding a Ti-Al composite. This surface data is required by gas phase transport simulations subsequently. The coupling of the two models needs to be realized via an appropriate model interface.

In this work, such a model interface is established based on machine learning techniques using artificial neural networks. As a proof of concept, a multilayer perceptron network is trained and verified with this set of incident/outgoing distributions. An error analysis is carried out for the obtained training results and their quality is compared and discussed for different sets of hyperparameters. Specifically, the influence of network depth and width, activation functions, as well as regularization and early stopping is evaluated. It is demonstrated that the trained network is able to predict the sputtered particle distributions for unknown, arbitrarily shaped incident ion energy distributions. It is consequently argued that the trained network may be readily used as a machine learning based model interface, which is sufficiently accurate also in scenarios which have not been previously trained. For this application, the prediction time and the possibility for run-time evaluation in the frame of a Monte Carlo transport simulations are finally investigated. To conclude, it is discussed that the conceptual methodology may also be considered in cases with more complex surface and gas compositions encountered in reactive sputtering.

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