PiAI Seminar Series: Physics informed AI in Plasma Science
9:30-10:30, 18 March 2024 (CET)
17:30-18:30, 18 March 2024 (JST)
Web Seminar

Coupling high-fidelity simulation and machine learning to bridge the gap between plasma simulation and material properties in PVD coating equipment.

Adam Obrusník

PlasmaSolve Co., Brno, Czech Republic

This contribution describes a very practical exercise of combining first-principle simulations with a simple machine learning method with the aim to be able to predict material properties of a quaternary coating prepared in PVD (physical vapor deposition) plasma-coating equipment.

Conventional process modeling of plasma equipment can be divided into two groups - physics-driven, i.e. numerical solvers solving the Boltzmann kinetic equation (BKE) for various particle species or moments of the BKE, and data-driven, i.e. large databases of coating recipes and characterized material samples which are either interpolated in or used as training data for machine learning or even AI. There are also methods of molecular dynamics which can in theory predict film properties. Even though these methods are very powerful in discovery of new materials, their uptake by the industry has been limited, possibly due to computational concerns and unknown potentials.

Furthermore, both the physics-driven and data-driven approaches contain an inherent disadvantage. Physics modeling can nowadays provide accurate results with easily accessible inputs, it predicts only the properties of the plasma (density, temperatures, species' mole fractions) and not the coating properties. On the other hand, the data-driven methods can predict material properties as such but require large training datasets because the number of input features is high.

In this contribution, we describe a methodology that we use for predicting material properties based only on inputs that one would require for a physics simulation and on a small dataset of 8 characterized samples of $Ti_xAl_ySi_zN$. We demonstrate that the combined physics simulation + machine learning approach can capture the trends in atomic composition but also in intrinsic properties (hardness, residuals stress) of a coating grown in an industrial PVD coater.