PiAI Seminar Series: Physics informed AI in Plasma Science
10:00-11:00, 19 June 2023 (CEST)
17:00-18:00, 19 June 2023 (JST)
Web Seminar

Machine Learning Surrogate Models for Plasma-Surface Interactions

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The development and true understanding of plasma processes (e.g., sputter deposition, catalysis) relies on accurate descriptions of the plasma-surface interactions involved. The length and time scales of the two states of matter differ in orders of magnitude and, hence, render a holistic modeling approach impractical. This issue is commonly addressed by completing simulations dedicated to surface-facing plasmas with effective but oversimplifying surface models (e.g., lookup tables). Adequately complex surrogate models are conceptualized and validated in this work by pursuing a data-driven approach for the sputter deposition of metals and metal nitrides in Ar and Ar/N_2 discharges. The data for plasma-surface interactions at the target and generalized wall (i.e., target, substrate, thin film) are aggregated with TRIDYN and hybrid reactive molecular dynamics / time-stamped force-bias Monte Carlo simulations, respectively. The latter imposes a significant computational cost, which hinders the accumulation of relevant data set sizes. This issue is addressed by the formulation of a novel, randomized data generation scheme. The data is used to combine and train a variety of machine learning architectures (e.g., physics-separating artificial neural networks) to overcome obstacles such as the general discrepancy of simulations and experiments regarding information accessibility. The evolution of thin films during growth and accompanied particle emission are predicted with high physical fidelity for experimental process times of 45 minutes in merely 34 GPU hours. In contrast, atomic simulations would take more than approximately 8 million CPU years.

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Project-ID 138690629 - TRR 87, - Project-ID 434434223 - SFB 1461, and - Project-ID 445072286.