CAMT Seminar

"Machine learning plasma-surface interactions: from low to high fidelity surrogate models"

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Center for Atomic and Molecular Technologies (CAMT)
(A12 棟 1 階会議室) & Webex Link (hybrid)

Abstract

Many technological applications of low-temperature plasmas (LTPs) rely on the interaction of the plasma with the surrounding walls. Whereas plasma-surface interactions (PSIs) may be described by surface coefficients (e.g., emission), these are often effective, averaged over various physical processes. Detailed knowledge on the surface kinetics may be obtained by sophisticated diagnostics, modeling, or a combination. These are often limited due to acquisition or computational requirements. Moreover, a comprehensive understanding of LTPs and related PSIs must be inherently multi-scale. This holds specifically for plasma modeling, where a consistent description requires sub-models on individual levels. In this work, the applicability of machine learning surrogate models to depict PSIs is discussed in the context of metallic thin film sputter deposition. Different surface models are assessed in terms of quality and abundance of data, as well as reliable physical descriptors. Lower physical fidelity data based on the transport and range of ions in matter simulations provide insight into the steady surface state; higher physical fidelity reactive molecular dynamics data capture also the dependence of a changing surface state. Both data sets are exploited for the training of corresponding machine learning models. The applied model architectures – based on artificial neural networks – are reviewed and the resulting prediction metrics are assessed. It is concluded that the obtained data-driven surrogate models entail the fidelity of the original physical models. They allow for a reliable and consistent multi-scale model coupling at significantly reduced computational costs. Envisioned applications of this modeling procedure include different plasma processes, materials, and phenomena (e.g., plasma catalysis).

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(Host: Satoshi Hamaguchi Ext：7913)