CAMT Seminar

“Dynamic surface surrogate model trained on atomistic data of AlN sputter depositions”

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Date: October 26, 2022 (Wednesday) 11:00-12:00
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Center for Atomic and Molecular Technologies (CAMT)
(A12 棟 1 階会議室) & Webex Link (hybrid)

Abstract

Modeling plasma-surface interactions is an often encountered multi-scale and multi-physics problem. Stepwise solutions have been proposed by replacing the surface with machine learning surrogate models for non-reactive processes. However, their applicability is still limited due to missing time dependencies or computationally too demanding explorations of parameter spaces. These remedies are resolved in this work for the reactive sputter deposition of AlN by applying a novel combinatorial approach to establish an internal surface state, which may evolve in time. Surface processes are initially studied by means of hybrid reactive molecular dynamics / force-bias Monte Carlo simulations, utilizing a therefor derived charge transfer equilibration model and a revised COMB3 AlN potential. The results are used to train multiple ensembles of physics-constrained artificial neural networks, which form a dynamic surface surrogate model for a wide range of working conditions. This model can be readily coupled to plasma simulations and diagnostics to predict realistic wall interactions (with molecular dynamics fidelity) as well as the transient evolution of surfaces.

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(Host: Satoshi Hamaguchi Ext：7913)