CAMT Seminar

"The Elucidation of Cu-Zn Surface Alloying on Cu(997) by Machine-Learning Molecular Dynamics"

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Online
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Abstract

The structure and the formation process of a Cu-Zn surface alloy formed on Cu(997) were investigated by machine-learning molecular dynamics (MLMD). The force-field required in the MD simulations is built by means of Gaussian Process (GP) regression aided with an on-the-fly active learning scheme. The simulation reveals a detailed atomistic picture of the long-time scale formation of Cu-Zn alloy on Cu(997) surface which was intractable in experiments. The surface alloying is initiated at the terrace near the step edge, highlighting the importance of step edges in the surface alloying. The rationalization of alloying behavior is performed based on statistics and activation energies of various elementary events that occur during the simulations. The dominant alloying mechanisms are found to be hopping descend and exchange descend near the step edge.

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