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Simulation of nano-coating formation mechanics and properties with variability in substrate surface topology

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Coating deposition process and the mechanics associated with substrate interactions are an increasingly important subject of research that promises to deliver a plethora of improved material properties for a wide range of applications. The surface topology of the substrate plays an important role in the boundary layer formation and the associated mechanical and thermal properties. The simulation of this process on nanometer to micrometer scale allows for a better understanding and prediction of the material composition and properties at the interface. This work examines the variability in coating/substrate interactions, compound formation rates, bond formation on nanometer to micrometer scale under variable substrate surface topology. The simulation takes advantage of hybrid multi-scale simulation methodology to produce large-scale models that maintain high fidelity at the substrate/coating interface. The simulation study has shown significant correlation between the substrate surface topology and orientation as well as deposition droplet size and incident angle during the deposition process and the mechanical properties and chemical composition of the substrate/coating interface. The study has identified the most significant topology groups and their correlation with deposition compound size and incidence angle for deposition process of metallic compounds.

Biography

Jamal Zeinalov is a Founder of Atomic Works, a software development company specializing in simulation platforms for nanomaterials. He has over 10 years of experience in "Scientific and engineering simulation software development fields" and holds a Doctorate degree in Aerospace Engineering. His research interests include "Material characterization and properties at nanometer to micrometer scale, advancement of size and time scale of molecular simulations, development of field force potential and bond formation simulations, nanomaterial simulations for metallic, ceramic, carbon based and biochemical applications".

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