Atomistic Simulations of Texture Evolution in Thin Films

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Abstract

Texture evolution during thin film deposition process spans 15 orders of magnitude in time. This large span challenges rigorous modeling of such evolution at the atomic level. Combining ab initio, molecular dynamics, and Monte Carlo Poly, the atomistic simulator of texture evolution (ADEPT) provides a capability of simulating texture evolution at the atomic level and under realistic deposition rates. In this talk, I will present our recent implementations and simulations in grain nucleation and subsequent texture evolution.