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Texture and Microstructure evolution in PVD films of fcc metals using Molecular Dynamics ASIT RAIRKAR, JAMES ADAMS, Arizona State University — Metallic polycrystalline thin films are used in a plethora of applications including especially metallic interconnects for the microelectronic industry. Numerous researchers have attempted to investigate both theoretical and experimental aspects of grain growth, texture competition and microstructure evolution. However the exact atomistic mechanisms behind these phenomena are still unknown. We attempt to study atomic level mechanisms behind polycrystalline thin film growth using Molecular dynamics techniques. The basic idea is to deposit Aluminum atoms on an fcc Lennard-Jones type of substrate with varying interaction energies with the Aluminum atoms. This will enhance the understanding of mechanisms behind island formation, substrate wetting, facetting in nuclei. We also report the results of similar depositions on Bicrystals of <110> and <111> oriented Aluminum slabs which result in dominance of the <111> grains by twinning mechanisms. All the MD simulations will be carried out at elevated temperatures and high deposition rates. This helps compensate the surface diffusion rates for the atomsThe goal of this study is to provide input to our multi-scale film growth model called FACET and the future 3D version of it called FACET-3D.

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