Materials Science & Engineering Doctoral Defense

Nanostructural Self-Organization In Vapor-Deposited Alloy Films: A Phase-Field Approach

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Abstract

Physical vapor deposition (PVD) of phase-separating multicomponent alloy films generates a rich variety of unique self-organized nanoscale morphologies. However, our understanding of how the different material and process parameters influence the formation of these nanostructures is limited. My dissertation aims to bridge this gap by developing phase-field models that can predict an entire spectrum of nanostructures as a function of processing conditions and composition in multicomponent alloys under a set of material-specific constraints. Firstly, we developed a numerical model to simulate nanoscale phase-separation in codeposited immiscible binary alloy films. An investigation on the influence of deposition rates, phase fraction, and temperature, on the evolution of self-assembled nanostructures yielded many characteristic patterns, including well known morphologies such as the lateral and vertical concentration modulations, as well as some previously undocumented variants. We also developed a numerical model to simulate phase-separation in physical vapor deposited ternary alloy films. We studied the influence of deposition rate and composition on the evolution of self-assembled nanostructures and recorded many novel nanoscale morphologies. We then imposed material constraints such as elastic misfit due to lattice mismatch between the phases, grain boundaries formed in polycrystalline films, and the interplay of interphase and surface boundaries at the film surface. To this end, we developed phase-field models that incorporated these constraints and studied their role in altering the temporal and spatial characteristics of the evolving morphologies. We also investigated the formation of surface hillocks and the role of surface and interfacial energies in their evolution. By studying the changes in excess energies across the different deposition models, we established that, in addition to influencing the temporal and spatial characteristics of nanoscale structures in the films, these energies are also responsible for driving morphological transitions as the rate of deposition is increased.Insights gained from our computational studies will demonstrate the viability of our models in predicting experimentally observed morphologies and supplement our understanding of the various factors involved in driving phase separations and morphological transitions. In addition, our morphology maps will serve as templates for developing new pathways for morphology control in the manufacturing of PVD alloy films.

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