Microstructure Morphology and Concentration Modulation of Nanocomposite Thin Films During Physical Vapor Deposition

Abstract: Nanostructured thin-films are nowadays regularly used as coatings to serve specific mechanical, chemical, electrical, or optical functionalities depending on the application. The physical and chemical properties of these thin-films directly depend on the microstructural configurations generated during the fabrication process, typically through physical or chemical vapor deposition (PVD or CVD) techniques. Understanding the phase-ordering kinetics controlling the way these microstructures develop during the synthesis process is crucial to obtaining reliable and enhanced functionalities for these nanostructured thin-films.

In this presentation, I will go over how we used phase-field modeling in order to gain insights into the complex competing mechanisms during the growth process of nanocomposite thin-films. This mesoscale model accounts for the deposition of the incident vapor phase of a binary alloy onto a substrate, the surface interdiffusion and the subsequent spinodal decomposition in the resulting elastically inhomogeneous binary thin film. Using the simulation results, I will show how we can be used this modeling framework to guide the synthesis of various types of achievable spontaneous self-assembled microstructure morphologies. Our numerical findings corroborate experimentally observed microstructures across a broad class of materials systems and synthesis conditions. I will end this talk with some thoughts on new opportunities and challenges we face when designing novel thin-films.

This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science user facility operated for the U.S. Department of Energy. This work was also supported by a Laboratory Directed Research and Development (LDRD) program at Sandia National Laboratories. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525. The views expressed in this article do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

Bio: Dr. Dingreville's research expertise is at the intersection of computational material science, experimental materials science and emerging fields in integrated computational mechanics. He employs and combines various theoretical and computational techniques (molecular dynamics, cluster dynamics, phase field, mean field, data mining) to understand and characterize materials aging and performance in solid matter. His research emphasizes designing materials with enhanced functionality through understanding and control of interface and defect phenomena. His research strategy is built on “reduced order mesoscale models”, which enable insights into how computational materials science and engineering can be exploited as discovery tools for applications into technologies such as nanostructures or advanced alloys.