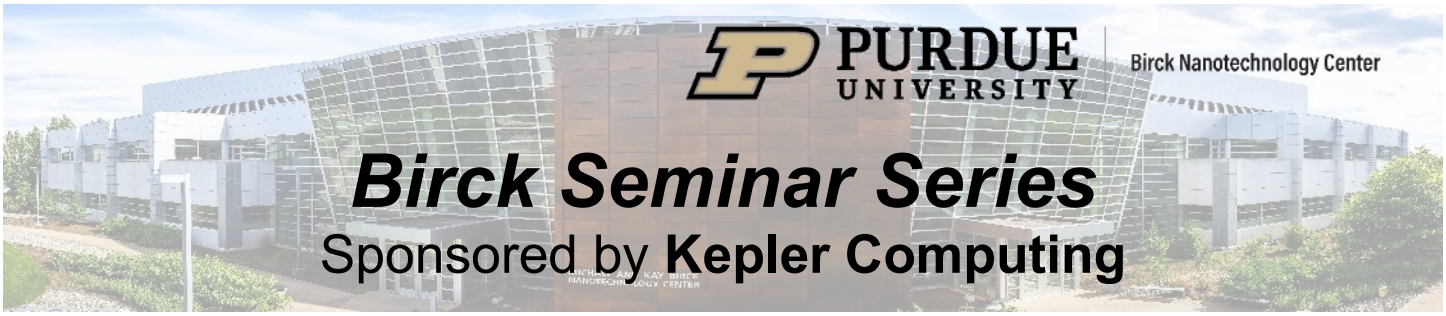

Computational Modeling of Pulsed Laser Deposition Growth of Multiphase Thin Films

Anter El-Azab

School of Materials Engineering

Wednesday, Sept. 10th @ 2:00 pm in BRK 1001

Coffee and snacks served before seminar

also on MS Teams

Abstract: Multiphase thin films grown via Pulsed Laser Deposition (PLD) technique have gained a significant attention in recent years due to their unique physical functionalities. In films with pillar-in-matrix configurations, vertical interfaces induce interesting physical, optical and chemical properties. Despite extensive experimental reports on multiphase film growth, a theoretical comprehension of the growth mechanisms and the influence of structure on properties is still lacking. In the case of growth morphology, it is known that both kinetic and thermodynamic factors are important but the relative roles of these factors are not yet understood. In this seminar, I will report on a recently developed multiscale computational capabilities of film growth developed by the Materials Theory and Data Science Group at MSE/Purdue. These capabilities are based on asynchronous, parallel kinetic Monte Carlo (kMC) simulation of film deposition and growth, informed by extensive Density Functional Theory (DFT) database of the fundamental properties of diffusion and bonding energetics and surface energetics, and augmented by continuum solution of the elastic strain arising from lattice and thermal mismatch in the heterogeneous film system. The elastic problem resulting from lattice and thermal mismatch between the substrate, matrix and pillar materials is cast in the form of Representative Volume Element (RVE) with average constraints and solved using Fast Fourier Transform (FFT). The kMC simulations reveal the impact of the PLD growth conditions on the film morphology. Furthermore, DFT investigations of the impact of strain on the bonding and diffusion of adatoms/molecules on the surfaces reveal that the local strain can play a significant role in the phase separation mechanism of oxide-metal systems and in the self-organization of phases on the substrate. The simulations are performed for Au-CeO2 film system deposited on SrTiO3 (001) substrate. Comparison with the experimental results will be given.

Bio: Anter El-Azab is a professor of Materials Science and Engineering at Purdue University. He obtained his doctorate degree in Engineering at the University of California, Los Angeles. Prior to coming to Purdue, he joined Pacific Northwest National Laboratory as a research scientist, and was a professor of Mechanical Engineering, Materials Science and Engineering and Computational Science at Florida State University. His current research focuses on the mechanics and physics of defects in materials and the influence of defects on materials properties. His latest research covers statistical modelling of dislocations and continuum dislocation dynamics, microstructure evolution in materials including thin films, radiation effects in nuclear materials, and coupled electron-phonon transport in defective solids via BTE. Part of his research is dedicated to the development of theoretical formalisms and computational and data science methods for multiscale and multi-physics modelling of materials, as well as the development of algorithms for bridging modelling and experiments in materials research.

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