

**MATERIALS ENGINEERING
SEMINAR**

“Interfacial Transitions and Microstructure Evolution of Materials”

By

Lucas Robinson

Purdue MSE Ph.D. Final Exam

Advisor: Professor Edwin García

ABSTRACT

In this thesis, a thermodynamically consistent phase field formulation was developed to identify the physical origin of interfacial transitions that drive macroscopic phenomena, starting at the single-particle length scale and building up to the polycrystalline length scale. At the single-particle length scale, the framework identified two interfacial phases that are stable at the surface of Sn nanoparticles: 1) a disordered interfacial phase, i.e., the experimentally observed premelted surface layer; and 2) an ordered surficial phase displaying a remnant degree of order in fully melted particles. Regimes of melting behavior as a function of particle size and temperature are discussed. To bridge the gap between single-particle and densified polycrystals, an analytical model was developed to capture the physical driving forces for densification during electric field-assisted sintering. Here, the model acknowledges the structural contributions of particle-particle interfaces to the strength of mechanical, electrical, and surficial driving forces for densification, and shows good agreement with experimental flash sintering data. Finally, the theory was applied to polycrystalline LiCoO_2 (LCO) and shows that the experimentally observed metal-insulator transition is driven by grain boundary lithium segregation, the interfacial misorientation, and the size of the abutting grains. A critical misorientation as a function of the macroscopic lithium content exists above which the grain boundaries undergo a metal-insulating transition, suggesting that the fabrication of textured LCO microstructures will delay the metal-insulator transition.

Date: Wednesday, March 8, 2023

Time: 10:00 A.M.

Place: HAMP 2107 or via Webex:

<https://purdue.webex.com/purdue/j.php?MTID=m350c60e09b77bee7d61c3b165c7b17ed>



School of Materials Engineering