MATERIALS ENGINEERING

SEMINAR

"Data Analytics on the Thermodynamics of $LiFePO_4$ Phase Field Modeling"

By

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ABSTRACT

This work aims to review the literature on experimental and numerical studies of $LiFePO_4$ (LFP). Experimental observations in LFP show two main phenomena: (1) the formation of solid-solution zone and metastable phases, and (2) the reduction in the miscibility gap with decreasing particle radius. Phase field models in the literature explain these two observations with different interpretations and implementations of the fundamental physics. There are two schools of thought in existing phase field models. One school interprets the experimental observation as a Crystalline-Disordered phase Transformation (CDT model), while another school interprets the observed phenomena as suppression of phase separation and elastic response of the material based on Surface-Reaction Limited model (SRL model). The limitations of the two models (CDT and SRL models) are discussed, along with recent advances in thermodynamic modeling of LFP that put into question the thermodynamic validity of these two. A new LFP phase field framework is proposed to address the limitations of current LFP phase separation models. Using the proposed framework, a phase field calculation of polycrystalline LFP phase separation that captures metastable phases reported in literature is presented. With a new approach in machine learning based phase diagram modeling from literature, the data analytics of LFP phase field models is explored by assessing the effect of different Gibbs free energy density functions.

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Time: 2:30pm
Place: HAMP 2118 or via
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