MAE *Faculty Candidate* Seminar

Phase-field simulations: A Tale of Two Materials

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206 Furnas

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ABSTRACT

The recent development in computational materials science has enabled "Materials-by-Design". This presentation will discuss the applications of mesoscale phase-field method to understanding and designing topological polar states in oxide heterostructures and understanding of dendrite growth mechanism in lithium metal anodes. As an example, phase-field simulations are employed to evaluate the geometric length scales that are critical for the formation of ordered polar vortex lattice in PbTiO3/SrTiO3 superlattice [1]. It is also discovered that switching of the vortex state will produce other transient polar states such as skyrmions, reminiscent of the Plateau-Rayleigh instability [2]. Further, it is predicted that polar skyrmions can be stabilized under zero applied field by compressive strain, which has been verified by experimental observations [3]. The properties of the topological structures are investigated, showing local negative capacitance that boosts the overall dielectric response of the thin film [4]. In another example, a nonlinear phase-field model is built to investigate the dendrite growth mechanism in lithium-ion battery with high capacity metal anode [5]. It is discovered that an intimate, dynamic competition between ionic transport and electrochemical reaction results in vastly different growth patterns. A step further, this model is extended to incorporate an energy balanced equation to account for the self-heating during high rate charging [6]. It is revealed that self-heating could accelerate/deaccelerate the dendrite growth in lithium metal anode, depending on the relative magnitude of ionic diffusion barrier and electrochemical reaction barrier.

[1] Z. Hong, et al., Nano Lett. 17(4), 2246 (2017).
[2] Z. Hong, et al., Acta Mater. 152, 155 (2018).
[3] S. Das, et al., Nature 568, 368 (2019).
[4] A. Yadav, et al., Nature 565, 468 (2019).
[5] Z. Hong, et al., ACS Energy Lett. 3, 1737 (2018).
[6] Z. Hong, et al., ACS Energy Lett. 4, 1012 (2019).

BIO SKETCH

Zijian Hong is a postdoc research associate in the Department of Mechanical Engineering at Carnegie Mellon University, Pittsburgh, working with Prof. Venkat Viswanathan. His mainly research interests are in multi-scale modeling/design of complex materials systems, namely, functional oxide heterostructures and battery materials. He received his B.Sc. from Zhejiang University, Hang Zhou in 2010, M.S. from Tsinghua University, Beijing in 2012 and Ph. D. from The Pennsylvania State University, University Park in 2017 (advisor: Prof. Long-Qing Chen), all in the Department of Materials Science and Engineering. In particular, his Ph.D. works mainly involve simulation-based design of ferroelectric topological state of matter and phase transitions in functional oxides. While as a postdoc at CMU, he developed a nonlinear phase-field model to understand the dendrite growth kinetics in lithium-ion batteries with metal anodes, aiming to design electrolyte/electrode systems for safe batteries with high capacity metal based anodes. Dr. Hong has 20+ peer reviewed publications (including 3 in Nature and 2 in Nature Materials), 10+ conference presentations, and 500+ scientific citations. He has reviewed over 20 papers for leading journals such as Acta Materialia, npj Computational Materials, Advanced Theory and Simulations and Advanced Intelligent Systems, etc. He received the department travel award from the department of Materials Science and Engineering at Penn State in 2015. He is currently a member of MRS.

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