Special MIE Seminar

11:00 AM Friday, February 12, 2016

*****GITC 3710*****

First-principles Based Multiscale Multiphysics Approaches for Integrated Computational Materials Engineering

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Advanced materials play key roles in the technological developments in many disciplines such as aerospace engineering, bioengineering, mechanical engineering and more. In order to reduce the cycle from design to deployment of advanced materials, integrated computational materials engineering (ICME) seeks to build a new paradigm that links design and manufacturing via materials models at multiple length scales in a seamless and integrated computational environment. Advances in computational and experimental materials science and engineering offer the promise for the rapid exploitation and introduction of new materials concurrent with system design and engineering through this innovative framework.

In this seminar, the importance of the first-principles based multiscale/multiphysics framework to realize the ICME paradigm will be demonstrated. By providing a deeper understanding of the underlying physics of the materials and systems at various length scales, a physics-based, i.e. first principles-based, computational predictive model would allow us to interpret and control complex materials and system behaviors. In particular, full atomistic and coarse-grained molecular dynamics simulation will be employed to investigate the microscopic structure and thermomechanical properties of polyethylene polymer and epoxy resin systems. The inter- and intra- molecular interactions at the nanoscale will be seen to significantly alter the materials properties. A reduced order model and an atomistic-continuum bridging method will also be demonstrated to link the discrete nanoscale description to the continuum description in both hierarchical and concurrent multiscale framework. Finally, the application of phase field modeling to the addictive manufacturing process will be presented, and the existing challenges and future research directions to advance the ICME paradigm through the multiscale computational approaches will be discussed.

Biography: Dr. Fu received her Master's degree in materials science and engineering from the Institute of Metal Research, Chinese Academy of Sciences in 2009, and PhD degree in mechanical engineering from University of Pittsburgh in 2013. She conducted her postdoctoral studies at University of South Carolina and University of Colorado at Boulder. Dr. Fu's research interests lie in the area of computationally guided innovative materials design and manufacturing as well as atomistic-continuum multiscale simulation to realize the integrated computational materials engineering paradigm. Her work has been published in more than 20 peer-reviewed journals and conference proceedings.