KTH SOLID MECHANICS SEMINAR; Thursday, January 23rd, 13.15; KTH Solid Mechanics Seminar room

Sarah C. Baxter, "Mechanics based Mechanical Percolation in Nanocomposites"

Polymer nanocomposites are the focus of a great deal of research as a framework in which to design and optimize multi-functional materials. By including a nanophase in a polymer matrix, significant improvements in properties have been observed at uncharacteristically low volume fractions.

For mechanical properties it has been hypothesized that enhanced properties are the result of the effect of the formation of a matrix-filler interface region. This local effect is present in all composite materials, but because of the high surface area to volume ratio for nanoscale inclusions, the interface region in nanocomposites can constitute a significant third phase of the composite and may contribute to the enhanced stiffnesses observed in nanocomposites.

Experimental evidence of these mechanical effects is in the form of property-volume fraction curves that resemble the percolation curves, associated with the formation of connected microstructures, and so the effect is commonly referred to as mechanical percolation. However, classic micromechanics models, which describe the mechanics, do not capture this percolation-like response. Percolation models, based on a probabilistically defined percolation threshold where the microstructure forms a connected microstructure, do not include significant mechanics.

Dr. Baxter is a Professor in the Department of Mechanical Engineering in the College of Engineering and Computing, at the University of South Carolina. She received her MS in Applied and Computational Mathematics at the University of Minnesota, and her PhD in Applied Mathematics from the University of Virginia. Her expertise is in computational solid mechanics, and her research is focused in the areas of stochastic micromechanics and probabilistic mechanics.

This talk will present a modeling methodology that includes both a micromechanical and a probabilistic approach to modeling mechanical percolation in nanocomposites. Random microstructures are simulated within a Monte Carlo framework and effective elastic composite properties approximated for each microstructural realization. The ensemble results show the evolution of percolating microstructures in two and three-dimensional material models, demonstrating a mechanics-based origin to influence of an interface region on composite properties and its role in interface assisted percolation.

This novel approach is a reversal of the modeling paradigm in that, rather than using a percolation threshold to predict mechanical properties, mechanical properties are developed that predict a mechanics-based percolation threshold.

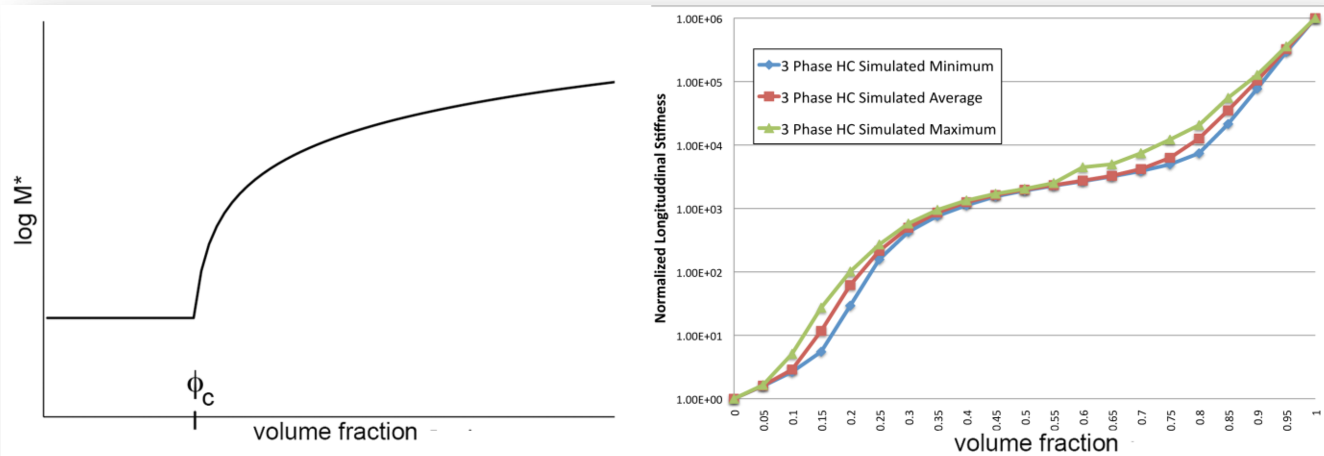

Figure at left shows the classice percolation curve based on threshold value ϕc. Figure at right characterizes a simulated percolation curve f or three dimensional nanocomposite with random microstructure. Low volume fraction percolation effects are due to interface assisted percolation, High volume fraction percolation is the result of a connected micrtostructure.