Mesoscale Networks:
from Microstructure Evolution to Material Properties

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Abstract: A major challenge in materials science is to understand and control the properties of materials based on the microstructure evolution at the mesoscale. For a wide range of materials, the relevant microstructures consist of a network of line objects. In this talk, I will use three examples to illustrate how the study of geometric/topological features of line networks can help us understand the microstructure-property relationship of materials.

The first example deals with dislocation line networks in crystals (such as metals) under plastic deformation. Over the last two decades, much effort has been placed on the prediction of stress-strain curve of single crystals through large-scale dislocation dynamics (DD) simulations. Our DD simulations reveal that the dislocation line lengths follow an exponential distribution in a dislocation microstructure of single crystal Cu under uniaxial loading along the [001] direction. A Boltzmann-type theory developed to explain this exponential distribution also reveals the new insights on the origin of strain hardening.

In the second example, we consider a coarse-grained molecular dynamics (CGMD) model of an elastomer in which the cross-link bonds can be broken. It is found that bond breaking caused by uniaxial loading does not occur at random locations in the polymer chain network. Instead they occur on shortest paths connecting far away beads (monomers). The evolution of the length distribution of shortest paths is found to control the stress-strain response of the elastomer.

The third example is concerned with a planar network of carbon nanotubes (CNTs) on an elastic substrate, acting as a stretchable electrode. The electrical resistance of the CNT network is measured during cyclic loading to progressively larger maximum strains. The hysteretic behavior of the resistance \( R \) as a function of strain \( \varepsilon \) is explained through the evolution of a microstructural parameter, \( \beta \), the relative coverage of single tubes, with strain. Analytical expressions are obtained for the relation between \( \beta \) and strain \( \varepsilon \), and between \( \beta \) and electrical resistance \( R \), which are consistent with both coarse-grained molecular statics (CGMS) simulations and experiments.

Biography: Wei Cai received his B.S. degree in optoelectronic engineering from Huazhong University of Science and Technology, P. R. China in 1995, and his PhD degree in nuclear engineering from Massachusetts Institute of Technology in 2001. He was a Lawrence Postdoctoral Fellow at the Lawrence Livermore National Laboratory from 2001 to 2004. He is currently an Associate Professor in the Department of Mechanical Engineering at Stanford University. He received the Presidential Early Career Award for Scientists and Engineers in 2004, and the American Society of Mechanical Engineers Hughes Young Investigator Award in 2013. His research interests include dislocation dynamics and metal plasticity, atomistic simulations of deformation, synthesis and transport mechanisms at the nanoscale. He is co-author of 95 journal publications in these and related fields, a book “Computer Simulations of Dislocations” (2006) and a undergraduate/graduate textbook, “Imperfections in Crystalline Solids” (2016).

Friday, 3/31/2017
12:00-1:00 PM
1610 Engineering Hall