Bridging Methods for Nano-scale Mechanics and Materials

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With the confluence of interest in nanotechnology, availability of experimental tools to synthesize and characterize systems in the nanometer scale, and computational tools widely accessible to model micro- and nanoscale systems with continuum/molecular/ quantum mechanics techniques, it vital to unravel the traditional gap between the atomic and the macroscopic world in mechanics and material science. This in turn opens up new opportunities in education and research. Traditional educators and researchers in mechanics and materials are well versed in continuum mechanics including topics such as elasticity, plasticity, dislocations, and fracture. As we evolve towards smaller and smaller components and systems, there is no doubt that we must move beyond continuum treatments and characterizations of mechanics and materials into the nanoscale. While most practitioners of mechanics and materials have been exposed to quantum mechanics at one time or another, such knowledge admittedly falls into disuse. This creates a significant barrier for most educators and researchers who wish to explore exciting new opportunities in nano mechanics and materials.

We will present multiscale bridging methods for micro-systems that couple molecular dynamics models with continuum models. Emphasis is placed on consistent treatment of the statistical behavior of the coupled model so that ensemble averages that determine state variables such as temperature and entropy are treated correctly. For these purposes, we use bridging scale models based on complete overlays. Methods for treating motion of dislocations across these interfaces will also be discussed. The methods will be applied to modeling of nanodevices and nanocoatings, and their use in the understanding of multi-physics of fracture and shear bands.

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