WCCM 2020 Minu-Symposium Abstract

Atomistic and Multiscale Modeling and Simulation of Nano- and Micro-structures of Materials and Their Applications

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Understanding material behaviors at macroscale is crucial in almost all engineering applications, and material behaviors are dictated by their material genomes, i.e. their nanoscale and microscale structures. Material microstructure is intrinsically a multiscale phenomenon, and the interaction among different scales can be either concurrent or hierarchical. Many mechanical and physicochemical characteristics of materials or their composites are at difference length/time scale, due to that the material property depends on the hierarchy of material internal structures. In microscale, different materials present significant differences in electron structure of atoms as shown by the periodic table of chemical elements. For meso-scale material systems, also they are controlled by the atomic and microstructures, the clusters of these structures, however, have different morphology and interatomic interactions. For assuring materials simulation across length/time scales, Multiscale modeling and simulation are essential to acquire in-depth knowledge for capturing the complicated behaviors of materials under different loading conditions and environmental conditions, such as plastic deformation, fracture, fatigue, radiation damage, size effect and surface effects, etc., because it can reveal the relationship between material macroscopic behavior and microstructure evolution.

Aiming at bring researchers from different disciplines working together on computational materials and computational physics, this mini-symposium will provide a forum for dissemination and discussion on recent research developments in first-principle modeling and simulations, multiscale analysis and methods that can be carried out to establish intrinsic relationships physically among different scales, focusing at exploring new approaches for designing materials or structures to satisfy specific and challenge requirements. We are interested in (but not limited with) those contributions on atomistic and multiscale modeling and simulations in various nano-materials and their applications, crystalline and metallic materials, energy materials, amorphous and ceramic materials, polymeric materials, biological and tissue materials, functional graded materials, smart materials, and various composite materials including civil engineering construction materials, etc.