ATOMISTIC, NANO, AND MICRO MECHANICS OF MATERIALS

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ABSTRACT

The underlying microstructure governs the macroscopic behavior of many materials, such as polymers, composites, or artificial metamaterials. Hence, nano and micro-scale effects must be explicitly modeled to capture these materials' behaviors and elucidate their structure-property relations.

To this end, a plethora of different modeling approaches have been applied to investigate such complex materials at different scales. These include ab initio methods, e.g., DFT, as well as particle-based methods such as molecular mechanics/dynamics, dissipative particle dynamics, and coarse-graining techniques for the atomistic and molecular scales. Furthermore, continuum approaches such as the finite element and finite different methods, fast Fourier transformation, peridynamics, and phase-field methods are employed to capture the intricacies at the microscale.

Additionally, many multiscale approaches have been developed to allow for a more holistic modeling of the materials or for a transition of findings from fine to coarse scale and vice versa. Examples are atomistic-continuum coupling (sequential, concurrent, hierarchical, and partitioned-domain) methods, as well as the heterogeneous multiscale method, quasicontinuum method, QM-MM, FE2, or FE-FFT.

This minisymposium invites scientists applying the aforementioned methods and aims to foster exchange on atomistic, nano-, and micromechanics across methods, scales, and disciplines.