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Multiscale Computational Methodology for the Mechanical Response of Nano- and Micro-Fiber Reinforced Cementitious Composites

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ABSTRACT

We propose a multiscale computational methodology to model the mechanical response of nano- and micro-fiber reinforced cementitious composites. The methodology is predicated by the idea that the overall response of the composite is controlled and optimized through molecular scale engineering of the chemical and mechanical interactions occurring at the material microstructure. The research particularly focuses on computational engineering of the reinforcement-matrix interfaces to achieve optimal mechanical and/or functional performance. In this work, a nonconcurrent multiscale approach is employed to link the scale of the material microstructure to the composite mesoscale (i.e., the scale of the representative volume), and a concurrent multiscale methodology is used to compute the overall behavior based on representative volume composition and response. The methodology provides a mathematically rigorous approach to incorporate interfacial atomic scale effects into continuum formulations.

The link between the chemical characteristics of the reinforcement-matrix interface (i.e., effect of functional groups) on the mechanical properties is established by the development of a nanoscopically informed cohesive zone model. The energy-based cohesive zone model provides the constitutive relationship between the cohesive tractions and relative motion of the constituents along the reinforcement-cement interface as a function of the interfacial chemical composition. The link between the chemistry and the interface cohesive energy is established based on molecular dynamics simulations of the material microstructure.

At the mesoscale, the representative volume element (RVE) of the cementitious composite is modeled as random short-fiber reinforced matrix, and the response is approximated based on the continuum formulation. An extended finite element method (XFEM) framework is proposed to evaluate the response of the RVE. By this approach, we eliminate the need of explicit resolution of each fiber within the RVE that leads to extremely complex finite element discretizations. Alternatively, the presence of the fibers is accounted for using additional enrichment functions that augments the standard finite element basis of a regular grid representing the cementitious matrix.

The overall (i.e., homogenized) behavior of the cementitious composite is computed based on the nonlinear computational homogenization theory with two spatial scales that span the meso- and macroscopic length scales.