

## MULTI-SCALE MODELING OF CEMENTITIOUS MATERIALS

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Advances in computational modeling are enabling the prediction and understanding of complex material systems, their properties and behavior through appropriate material models at different length scales, starting from the molecular scale material chemistry level to the micro, and macro scale level. These multi-scale models provide a paradigm for coupling material science, molecular chemistry level models into engineering design, and are expected to provide a detailed multi-scale understanding of complex material systems. Cementitious materials, an excellent example of highly heterogeneous material systems, are cement-based systems that include cement paste, mortar, and concrete; though commonly used are one of the most complex in terms of the material morphology and structure than most materials, for example, crystalline metals. Processes and features occurring at the nanometer sized morphological structures affect the performance, deformation/failure behavior at larger length scales. In addition, cementitious materials undergo chemical and morphological changes gaining strength during the transient hydration process. Hydration in cement is a very complex process creating complex microstructures and the associated molecular structures that vary. A fundamental understanding can be gained through nano to continuum multi-scale level modeling for the behavior and properties of cementitious materials from the material chemistry level atomistic scale to further explore their role and the manifested effects at larger length scales. These multi-scale material models further enable the understanding and influence of the material chemistry changes and nanomaterial additives on the expected resultant material characteristics and deformation behavior.

Multi-scale modeling of such material systems requires starting from the fundamental building blocks for the analysis and understanding at each of the disparate length scales capturing the scale relevant features through associated computational models. In conjunction, techniques to correlate across the morphological features at each of the length scales and the associated computational coupling techniques across the multiple scales are required. In this paper and presentation, recent work from our research group on the nano to continuum modeling of cementitious materials, in particular, cement paste will be discussed.

The presentation will emphasize on the computational modeling at different length scales building the foundations of our research work consisting of

- a) Molecular Dynamics modeling for the nanoscale features of the cementitious material chemistry. While most of MD analysis had been limited to stiffness predictions, our recent work on the computational material modeling of deformation and thermodynamic state effects needed in high strain rate behavior of cementitious material systems will be highlighted. Material chemistry level modeling allows one to understand the effect of material chemistry and additive changes on the stiffness and deformation characteristics.
- b) Micromechanics modeling employing the cement microstructure morphology that takes into account the variations in the morphological features will be discussed. The material morphology at the microstructure level consists of fundamental material constituents whose properties and behavior are strongly influenced by the molecular morphology of these material systems and their geometrical distribution.

Results and findings from our recent work on the scale relevant modeling of the multi-scale heterogeneous cementitious materials will be presented to further providing a forum for technical interactions and collaborations on the current state of the art, technology and research coupling material science and engineering that is essential in multi-scale modeling.