Material Chemistry Level Deformation and Failure in Cementitious Materials

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Abstract : Cementitious materials, an excellent example of highly complex, heterogeneous material systems, are cement-based systems that include cement paste, mortar, and concrete that are heavily used in civil infrastructure; 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 with hydration. A fundamental understanding can be gained through multi-scale level modeling for the behavior and properties of cementitious materials starting from the material chemistry level atomistic scale to further explore their role and the manifested effects at larger length and engineering scales. This predictive modeling enables the understanding, and studying the influence of material chemistry level changes and nanomaterial additives on the expected resultant material characteristics and deformation behavior. Atomistic-molecular dynamic level modeling is required to couple material science to engineering mechanics. Starting at the molecular level a comprehensive description of the material's chemistry is required to understand the fundamental properties that govern behavior occurring across each relevant length scale. Material chemistry level models and molecular dynamics modeling and simulations are employed in our work to describe the molecular-level chemistry features of calcium-silicate-hydrate (CSH), one of the key hydrated constituents of cement paste, their associated deformation and failure. The molecular level atomic structure for CSH can be represented by Jennite mineral structure. Jennite has been widely accepted by researchers and is typically used to represent the molecular structure of the CSH gel formed during the hydration of cement clinkers. This paper will focus on our recent work on the shear and compressive deformation and failure behavior of CSH represented by Jennite mineral structure that has been widely accepted by researchers and is typically used to represent the molecular structure of CSH formed during the hydration of cement clinkers. The deformation and failure behavior under shear and compression loading deformation in traditional hydrated CSH; effect of material chemistry changes on the predicted stress-strain behavior, transition from linear to non-linear behavior and identify the on-set of failure based on material chemistry structures of CSH Jennite and changes in its chemistry structure will be discussed.

Keywords : cementitious materials, deformation, failure, material chemistry modeling
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