

Computational Material Chemistry Level Modeling of Materials – Cement Paste

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Abstract

Cementitious materials (cement paste) are highly heterogeneous and hierarchical material systems. Processes and features at the nanometer sized morphological structures affect the performance, deformation/failure behavior at larger length scales. Further, cement paste undergo chemical and morphological changes gaining strength during transient hydration process. Mechanical properties, deformation and failure are thus influenced by starting material genome chemistry structures, their evolution to microstructures and engineering scale.

Molecular Dynamics (MD) modeling methods built upon material chemistry level molecular models provide a viable methodology to study and characterize material systems based on nanoscale and chemistry level features. The present paper presents our work on the material modeling of deformation and failure of nanoscale hydrated calcium silicate hydrate (CSH) in cement paste. In particular, MD modeling shear and compression deformation of hydrated cement paste constituent calcium-silicate-hydrate (CSH) is discussed. Computational CSH molecular structure (Jennite) is subjected to shear and compressive deformation resulting in the predicted shear stress - strain behavior along its main crystalline orientations, and an estimation of shear modulus and strength.

In the case of shear deformation, simulation results indicated that the nanoscale CSH Jennite under shear deformation displays a linear elastic behavior up to shear stress of approximately 1.0 GPa, and shear deformation of about 0.08 radians, after which point yielding and plastic deformation occurs. The shear modulus determined from the simulations was 11.2 ± 0.7 GPa. The deformation-induced displacements in molecular structures were analyzed dividing the system in regions representing calcium oxide layers. The displacement/deformation of the layers of calcium oxide forming the structure of nanoscale CSH Jennite was analyzed. The non-linear stress-strain behavior in the molecular structure was attributed to a non-linear increase in the displacement due to sliding of the calcium oxide layers on top of each other with higher shearing. These results support the idea that by controlling the chemical reactions, the tailored morphologies can be used to increase the interlinking between the calcium oxide layers, thus minimizing the shearing of the layers and leading to molecular structures that can withstand larger deformation and have improved failure behavior.

In addition, recent results from compression deformation, material chemistry changes and macro-molecular systems with multiple cement material phases emulating the material scale and features captured in nanoindentation will be discussed.

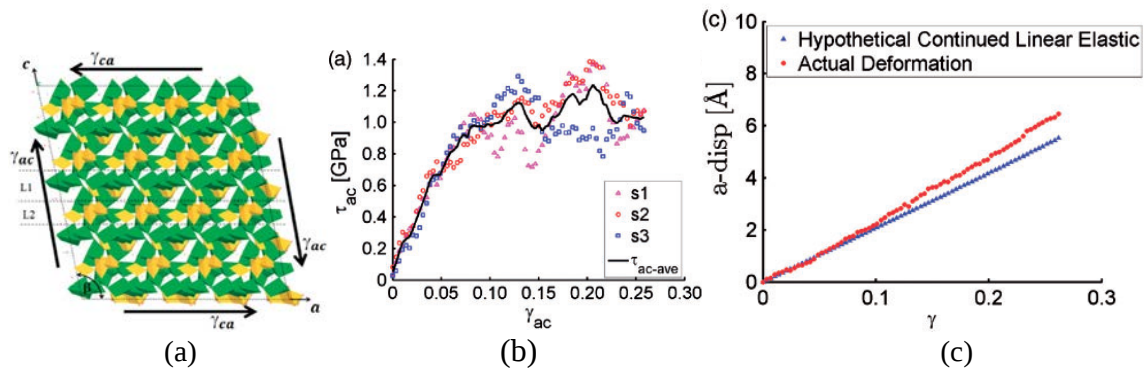


Figure 1. Shear deformation of nanoscale CSH Jennite: (a) Molecular structure (b) Shear stress – strain deformation (c) Linear to non-linear deformation and failure analysis