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Shock Wave Propagation in Cementitious Materials at Micro/Meso Scales

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The mechanical and constitutive response of materials like cement, and bio materials like fish scale and abalone shell is very complex due to heterogeneities that are inherently present in the nano and microstructures. The intrinsic constitutive behaviors are driven by the chemical composition and the molecular, micro, and meso structures. Therefore, it becomes important to identify the material genome as the building block for the material. For instance, in cementitious materials, the genome of C-S-H phase (the glue or the paste) that holds the various clinkers, such as the dicalcium silicate, tricalcium silicate, calcium ferroaluminates, and others is extremely complex. Often mechanical behaviors of C-S-H type materials are influenced by the chemistry and the structures at all nano to micro length scales. By explicitly modeling the molecular structures using appropriate potentials, it is then possible to compute the elastic tensor from molecular dynamics simulations using all atom method. The elastic tensors for the C-S-H gel and other clinkers are determined using the software suite "Accelrys Materials Studio." A strain rate dependent, fracture mechanics based tensile damage model has been incorporated into ABAQUS finite element code to model spall evolution in the heterogeneous cementitious material with all constituents explicitly modeled through one micron element resolution. This paper presents results from nano/micro/meso scale analyses of shock wave propagation in a heterogeneous cementitious material using both molecular dynamic and finite element codes.