# Nano-Scale Investigation of Failure Mechanisms in Al-Rich Species of Hydrated Cement Paste Subjected to Extreme Deformations

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## I. Introduction

- Application 1: The Al-rich species constitute up to 15 wt.% of cement paste.
  Issue: Early Ettringite Formation (EEF) and Delayed Ettringite Formation (DEF) that cause undesirable cracking and deterioration of cement-based materials.
- Application 2: The Al-rich species are used as a binder for hazardous waste encapsulation.
  Issue: Strength requirement for efficient stabilization of heavy ions.

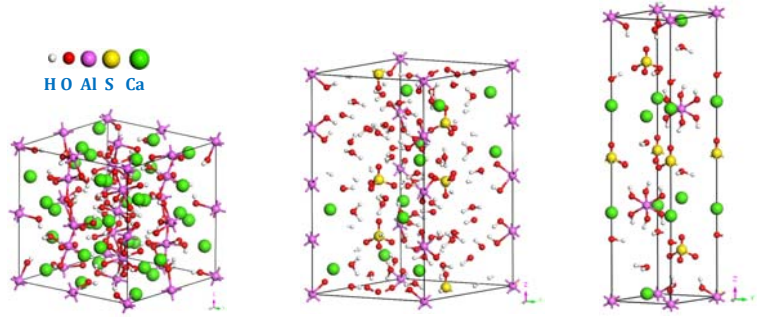
## II. Motivations and Objectives

- Interpret the findings at large length scales based on the structural response and failure mechanisms that occur at the nano-scale.
- Understand the mechanical properties of the Al-rich species that are detrimental to control the strength development in a range of common cementitious materials.

## III. Methodology: Atomistic Simulation

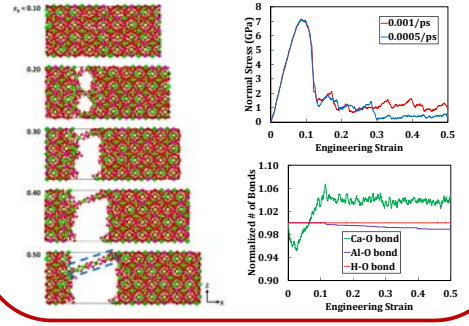
- Initialization: Setup atomistic model; define initial atomic positions and velocities; define reactive force field (ReaxFF); energy minimization
- Reactive Molecular Dynamics: Calculate forces; update atomic positions and velocities, iterate until thermodynamic equilibrium is reached
- Uniaxial Tension Straining: Strain simulation cell in a Cartesian direction; remap positions of atoms; relax lateral directions, repeat until permeant failure occurs
- Post-Processing: Collect trajectories, determine stress-strain relationships

## IV. Atomistic Models of Al-Rich Species of Hydrated Cement



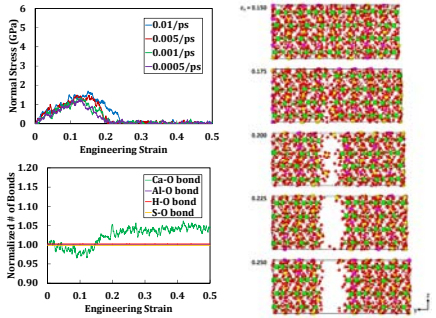

## V. Hydrogarnet: Failure Mechanism

✓ In *x*, *y*, and *z* directions:

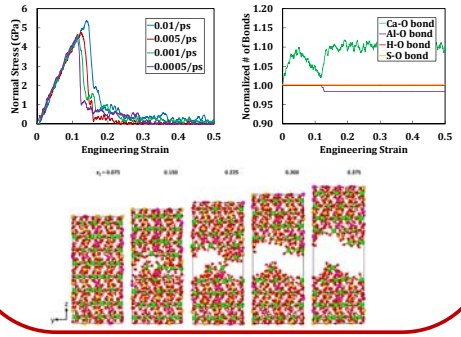



## VI. Ettringite: Failure Mechanisms

✓ In *x* and *y* directions:



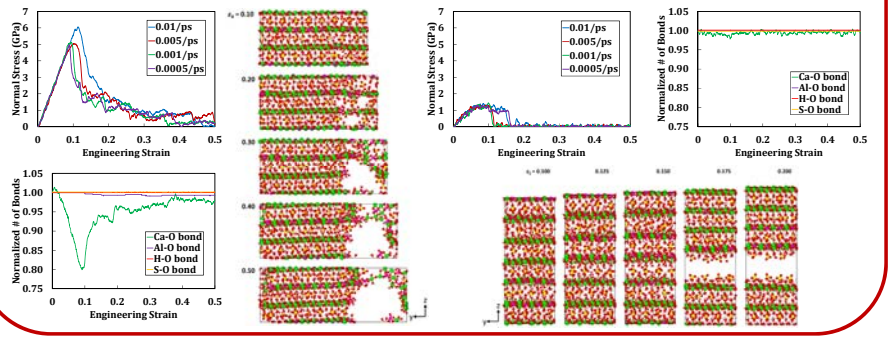

✓ In *z* direction:




## VII. Monosulfoaluminate: Failure Mechanisms

✓ In *x* and *y* directions:

✓ In *z* direction:




## VIII. Conclusions and Future Works

✓ The presented results are expected to directly contribute to understand how the strength and stiffness of the Al-rich species of hydrated cement can be improved based on the fundamental mechanical behavior captured at the atomic scale.

| Species | Dependency | | Strongest Component |
|---|---|---|---|
| | Strain Rate | Directions | |
| Hydrogarnet | ✓ | × | Ca-O and Al-O Bonds |
| Ettringite | ✓ | ✓ | Tricalcium Aluminate Columns |
| MonSAl | ✓ | ✓ | Calcium Aluminate Layers |