National Institute of Technology Rourkela

Departmental Seminar

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| Seminar Title | : Conference Return Seminar: Molecular dynamics simulation of edge crack propagation in CSH gel under direct bending |
| Speaker | : Dr. Sonali Bhowmik |
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| Venue | : Civil Engineering Seminar Hall |
| Date and Time | : 27 Sep 2024 (03:00 PM) |
| Abstract | : Comprehending the fracture behaviour of concrete is a difficult task due to its multiscale heterogeneous structure at different length scales, extending from nanoscale to macroscale. The Calcium Silicate Hydrate (CSH) gel is the major binding phase in concrete structures, responsible for the overall mechanical and fractural strength. At atomic scale, interaction of CSH gel under different loading conditions can provide insights into the fracture process of concrete. To study load resistance capacity of CSH gel, a molecular dynamics case study has been performed here. The reactive molecular dynamics methods are employed to study the atomic breakage in CSH using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). The CSH gel is subjected to three-point bending under static loading. For the simulation of bending behaviour, the ends of the CSH gel are clamped along y-axis and the load is perpendicularly applied in z-direction. An inherent defect is introduced in the material to simulate the crack propagation behaviour in the mentioned loading conditions. All the tests have been carried out at room temperature (300 K) and atmospheric pressure. During, the application of load, non-periodic boundary conditions are applied in all three directions, to get an isolated system. And the effect of loading has been studied by means of fracture toughness and crack opening displacements for the specified edge-cracked specimen. The bending behaviour of CSH gel has been successfully simulated by the molecular dynamics study. The present analysis sheds light on the role of different bonds in the crack resisting behaviour. The obtained results aid in improving the understanding of various toughening mechanisms happening at atomic scale. Thus, providing a basis for an optimised design at macroscale. The fracture properties obtained from this study can further be used as an input for continuum length scales models. |