
Departmental Seminar

Seminar Title	: Conference Return Seminar: Effect of notch size and orientation on the fracture of concrete interface: an MD simulation study
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Venue	: CE Seminar Hall
Date and Time	: 02 May 2025 (04:00pm)
Abstract	: Concrete interfaces between aggregates and cement paste are critical zones for crack initiation and propagation. At nanoscale, the interface between Calcium Silicate Hydrate (CSH) and silica is crucial as its cracking significantly affects the structural performance. In this study, classical Molecular Dynamics (MD) simulations are employed to examine the crack growth mechanisms in notched specimens under Mode-I loading. The effect of notch size and its orientation on the fracture behaviour of CSH-silica interface is explored through reactive MD. The interface is characterized by atomic-level interactions, stress distribution, and energy dissipation, providing substantial insights into the fracture toughness and crack propagation. The study highlights the key aspects of atomic debonding, crack initiation and growth. Thus, contributing to a deeper understanding of the mechanical integrity and fracture resistance of cementitious materials. The results reveal that the larger notch size and unfavourable orientations lead to accelerated crack propagation and reduced fracture resistance. While smaller or optimally oriented notches enhance the specimen's ability to withstand the applied stresses. These findings contribute to a better understanding of fracture mechanics in concrete at the nanoscale and offer valuable guidance for optimizing concrete design for improved durability and performance.