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EFFECT OF NOTCH SIZE AND ORIENTATION ON THE FRACTURE OF CONCRETE INTERFACE: AN MD SIMULATION STUDY

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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.

1 INTRODUCTION

Concrete is a multiphase material exhibiting complex fracture behavior due to its microstructural heterogeneity and quasi-brittle nature. The role of inherent heterogeneity and microstructural defects on the macroscale fracture behavior have garnered significant research interests as cracks weaken the load-bearing capacity and shorten the service life of concrete structures. While significant advancements have been made in understanding concrete's fracture at the macroscale, investigating this phenomenon at the nanoscale has become increasingly essential for a more comprehensive understanding. At the nanoscale, the fracture process begins with the breaking of chemical bonds. Among the various cement hydration products, the Calcium Silicate Hydrate (CSH) gel is the backbone of concrete's binding matrix. As the most abundant phase, it's properties are representative of mortar and governs the overall mechanical and durability properties. Despite its significance, understanding the fracture behavior of C-S-H gel remains a complex challenge due to its nanoscale heterogeneity, disordered structure, and multiscale interactions. These complexities necessitate advanced methods to investigate its fracture mechanisms at the atomic level, where traditional experimental techniques face significant limitations.

Molecular Dynamics (MD) simulations have emerged as a powerful tool to study the fracture behavior of CSH gel at the nanoscale. MD provides an atomistic perspective, enabling researchers to analyze the breaking of chemical bonds, the formation of nanoscale cracks, and the redistribution of stress during fracture. This computational approach complements macroscopic and microscopic studies by offering insights into the fundamental mechanisms that drive crack initiation and propagation, which are critical for predicting the macroscopic performance of concrete.

Pellenq et al. [1] in their groundbreaking work proposed a tobermorite based CSH model with a stoichiometry of $(CaO)_{1.65}(SiO_2)(H_2O)_{1.75}$ using MD. Incorporating this method, various studies have reported the use of MD in estimating various structural and mechanical properties of CSH gel under different conditions [2, 3]. Hou et al. [4] employed MD simulations to study the mode I fracture in CSH gel under direct tension loading. It was revealed that at the nanoscale, the layered CSH gel exhibits a dual behavior in crack propagation. Within the xy plane, the stable ionic-covalent Si–O and Ca–O bonds resist breaking, slowing the coalescence of cracks and reflecting a ductile nature. Conversely, along the z direction, cracks propagate rapidly through the interlayer regions due to the frequent breaking of the H-bond network, indicating a brittle behavior. Similarly, Bauchy et al. [5] used molecular dynamics simulations to study the fracture toughness of CSH, offering key insights into the mechanisms of crack propagation and the role of microstructure on fracture resistance. They confirmed the inapplicability of Linear Elastic Fracture Mechanics (LEFM) based methods in determining the fracture toughness and energy of CSH gel due to its ductile failure. A study by Wu et al. [6] emphasized the role of strain rates in the tensile strength of CSH gel. The results reveal the enhancement of mechanical properties at higher strain rates.

The interface plays a pivotal role in determining the mechanical properties and overall performance of concrete. The nanoscale interactions between C-S-H gel and other phases, including aggregates and the interfacial transition zone (ITZ), critically influence the macroscopic properties of concrete. This region often exhibits unique structural and chemical characteristics that significantly influence crack propagation, stress distribution, and bonding strength. The study by Kai and Dai [7] explores the atomic-level interfacial characteristics between geopolymer binders and silica aggregates, focusing on three typical Si/Al ratios of the geopolymer. Here, the interfacial strength is evaluated using a strain-controlled method, capturing the complete fracture process. The nanoscale interfacial characteristics between cement paste and silica remain poorly understood. In this regard, Kai et al. [8] uses molecular models to investigate the interactions between CSH and silica. The interfacial structures were characterized and fracture process revealed three stages: crack propagation, atomic chain bridging (contributing to residual strength), and complete failure. These findings pave the way for studying the atomic-level interfacial interactions mechanisms.

Microcracks and notch size play a crucial role in determining the fracture behavior and mechanical properties of CSH gel. At the nanoscale, these defects serve as initiation points for crack propagation, influencing the material's toughness, ductility, and failure mechanisms. These nano-defects play a key role in determining the strength of cementitious composites across their hierarchical structure [9]. Cao et al. [10] used MD simulations to examine the effects of pore size and fatigue loading on NaCl transport in CSH nanopores. It was revealed that chloride ions are attracted to the pore walls by adsorbed Ca^{2+} and Na^{+} ions and as the pore diameter increases, the attractive interaction between the pore walls and chloride ions becomes weaker. Zhang and Shahsavari [11] showed that the introduction of voids and portlandite particles significantly enhances toughness and ductility, particularly in C-S-H

with highly amorphous matrices. This improvement arises from competing mechanisms, including crack deflection, void coalescence, internal necking, and adjustments in void/particle geometry, which collectively balance toughness and strength. Liang [12] studied the role of crack size in the fracture of CSH-CH (Calcium Hydroxide) composite. It was revealed that the crack primarily propagates near the interface and within the C-S-H phase due to the weak hydrogen bonds in its interlayer region. As the crack width increases from 0 Å to 28 Å, the maximum reductions in uniaxial tensile strength and Young's modulus are 20% and 22%, respectively, indicating that cracks significantly affect the mechanical properties of the CSH-CH composite.

Even though MD simulations have been actively used in studying the nanoscale behavior of CSH gel, the behavior of other interfaces, such as those between aggregates and cement paste, has not been addressed fully. A broader investigation into various interfacial mechanisms from the perspective of crack propagation is necessary. In this study, a MD simulation study has been performed by considering the effect of notch size and orientation on the fracture performance of the CSH-silica interface.

2 SIMULATION FRAMEWORK

2.1 Construction Methodology

As sand is the primary chemical component in aggregates, a silica (SiO_2-alpha) unit is used here to create a representative aggregate model. The unit cell dimensions of monoclinic silica cell are: 4.91 x 4.91 x 5.41 Å with $\alpha = \beta$ as 90° and γ as 120°. Initially, a silica supercell with dimensions of 11 × 18 × 17 times the unit cell is converted into an orthorhombic structure measuring 54.04 × 76.58 × 86.88 Å. Subsequently, two exposed silica surfaces were generated by attaching hydrogen (H) atoms to the exposed oxygen (O) atoms on the top and bottom surfaces, forming a hydrated surface layer (Si-OH) [8]. Afterwards, amorphous CSH molecular models were then constructed and positioned in contact with the silica surface. The CSH unit cell data was taken from Zhang et al. [13] with dimensions as: 27.5 x 38.0 x 22.9 Å and α = 92.3°, β = 88.5°, γ = 88.3°. The presence of hydrogen atoms on the silica surface facilitates the CSH bonding, forming a composite structure at the interface.

2.2 Simulation Steps

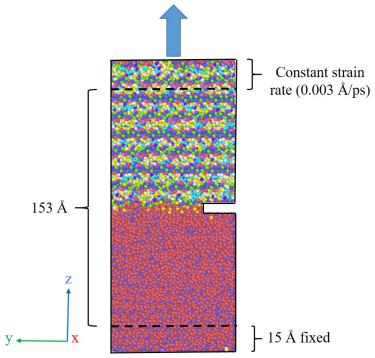


Figure 1: Schematic respresentation of loading details. (Colour indices- Silica: Burgundy represents Oxygen (O), Navy blue represents Silicon (Si), Yellow represents Hydrogen (H); CSH: Purple represents Silicon (Si), Green represents Calcium (Ca), Violet represents Oxygen ions, Sky Blue represents Hydrogen (H), Blue represents Oxygen atoms (O))

The obtained CSH-silica interface model was first geometry-optimized through energy minimization using the Conjugate Gradient (CG) algorithm with convergence criteria set to 10^{-6} kcal/mol for energy and 10^{-6} (kcal/mol)/Å for force. This was followed by establishing thermodynamic equilibrium over 500 ps (picoseconds) in an isothermal-isobaric (NPT) ensemble maintaining a temperature of 500 K and a pressure of 101 kPa (atmospheric pressure). This thermal treatment facilitated the acceleration of chemical and physical processes within the interfacial structures. Following this, the systems were cooled to 300 K (room temperature) at a cooling rate of 10 K/ps. They were then equilibrated for an additional 300 ps in an NPT ensemble, maintaining a temperature of 300 K and a pressure of 101 kPa. The over-

all equilibrium of the system was performed at periodic boundary conditions.

The investigation of fracture processes are done by applying uniaxial tension force in the z-direction with fixed boundary conditions. The loading procedure involved constraining the lower regions (z-coordinates less than 15.0 Å) while applying a constant velocity of 0.003 Å/ps to the upper regions (z-coordinates greater than 168.6 Å). Before applying load, the defects of sizes 11 x 8 Å, 15 x 8 Å and 20 x 8 Å were introduced in y-z axis to study the fracture behavior at different notch sizes. The schematic representation of the loading details with an initial notch is shown in Fig. 1. To study the effect of notch orientation on the interface model, the initial void of 15 x 8 Å is introduced seperately in CSH gel and silica also. This will provide an elaborate effect of inherent voids in the crack propagation of concrete. The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [14] was utilized for all simulations, employing a timestep of 0.01 femtoseconds (fs).

2.3 Force Field

The present study employs the reactive force field (ReaxFF), developed by Duin et al. [15], to capture both inter- and intra-molecular interactions within the molecular structure. Unlike traditional force fields, ReaxFF employs a bond-order-dependent energy formulation, allowing dynamic changes in bonding environments to be captured seamlessly. Consequently, ReaxFF enables the accurate modeling of chemical bond formation and dissociation, making it particularly suitable for studying the complex behavior of CSH gel under mechanical stresses [8]. The total potential energy in this force field is represented as:

$$E_{system} = E_{over} + E_{under} + E_{bond} + E_{val} + E_{lp} + E_{H-bond} + E_{torsion} + E_{vdWal} + E_{Cb} \quad (1)$$

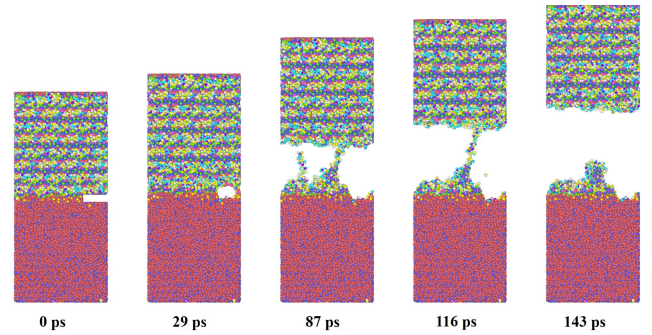
where E_{over}, E_{under} are the energy penalties for over and under-coordination of atoms, respectively. E_{bond} is the bond energy representing bond formation and dissociation. E_{val} is valence angle energy and E_{lp} is lone pair energy. $E_{H-bond}, E_{torsion}$ are hydrogen-bond and torsion angle energies, respectively. E_{vdWal}, E_{Cb} are the van der Waals energy describing non-bonded interactions and coulombic energy accounting for electrostatic interactions between partial charges, respectively.

3 RESULTS AND DISCUSSIONS

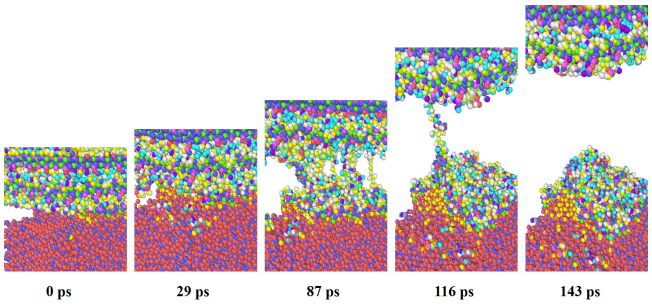
The molecular configuration of the damaged structure can provide deeper insights into the heterogeneous behavior at the atomic scale. In this section, the outcomes of the MD simulations are presented to explore the influence of notch size and orientation on the fracture behavior of concrete interfaces. Fig. 2 shows the atomic snapshots of the specimen with an initial crack size of 20 x 8 Å at different timesteps, using OVITO software [16]. The simulation is executed until complete rupture of interface occurs, after which it is terminated. Fig. 2 (a) shows the dynamic evolution of the fracture process at the interface from the left alignment, while an enlarged perspective view is presented in Fig. 2 (b). The periodic boundary condition applied in the y-direction of the simulation box causes atoms to re-enter, giving the illusion of crack closure at the 29 picoseconds (ps) timestep. However, these atoms are non-bonded and do not have an impact on the crack propagation. As time progresses, the interface begins to separate with atomic crack bridging occurring prior to complete fracture. From the perspective view of the interface, it can be observed that at nanoscale, the fracture in concrete is more ductile, aligning with the observations of Bauchy et al. [5] and the atomic breakage does not follow a regular path. During elongation, the atomic separation initiates at both ends and chain bridging primarily occurrs in the middle. The crack predominantly propagates through the CSH layer nearby the interface due to presence of weak hydrogen bonds in CSH. With the progression of load, the CSH layer detaches from the silica unit, leaving behind some CSH particles on the interface.

The visual inspection of fracture simulations

with varying notch sizes revealed that larger initial notches result in earlier failure compared to other models. At the same time interval, the model with a 20 x 8 Å crack size begins to exhibit atomic chain bridging, whereas the 11 x 8 Å model shows only minor void formation. These microvoids undergo cycles of spontaneous bonding and de-bonding, contributing to energy dissipation and fracture toughening. The effect of chain bridging is also most pronounced in the 11 x 8 Å notch model, followed by the 15 x 8 Å and 20 x 8 Å models.



(a)



(b)

Figure 2: Atomic snapshots of the fracture of cracked interface (a) left, (b) perspective view.

Notches in MD are a representative of microstructural defects and often play a significant role in the initiation and propagation of cracks. In heterogeneous materials like concrete, microcracks are randomly distributed within the structure. To gain further insights on the role played by different notch orientations on the overall fracture behavior, a detailed study is conducted by introducing initial notches in CSH and silica, respectively. Fig. 3 shows the atomic snapshots of the fracture simulations for interface models with initial cracks located in CSH. From the visual inspection, it was observed that the presence of initial notch in CSH facilitates the crack propagation due to the disruption of interlayer hydrogen bonds. This model exhibits the fastest complete rupture among all interface models, with no observable necking. Additionally, the contribution of atomic chain bridging to the fracture mechanism is minimal in this configuration.

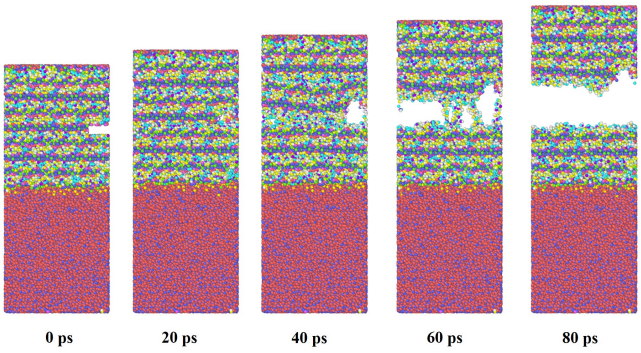


Figure 3: Atomic snapshots of the fracture of interface with initial notch in CSH.

The simulation of fracture for the interface model with an initial crack in silia is depicted in Fig. 4. It is interesting to observe that even though the notch is present in silica, the fracture starts from the interface only. The strong covalent bond between silicon and oxygen in Si-O-Si skeleton and its high bond dissociation energy contributes to a stable structure and provides higher resistance to mechanical degradation. This conforms with the fact that interface is weaker in the hardened concrete and crack is likely to propagate in mortar matrix or interfacial transition zone. The probability of aggregate rupture in large scale concrete structures is very low as also reflected in the MD simulation results. Furthermore, for the interface model with an initial notch in silica, the overall fracture behavior resembles that of an un-notched specimen.

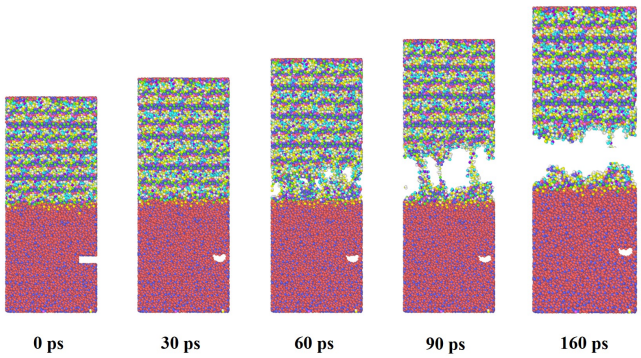


Figure 4: Atomic snapshots of the fracture of interface with initial notch in silica.

To further investigate the mechanical and fracture response of the interface model with varying notch sizes and orientations, the load-deformation curves are plotted. Fig. 5 represents the response of cracked interface for various notch sizes. The deformation is in Angstorms (Å) and the load is in nanonewtons (nN). For all three notch sizes, there is a linear increase in load with deformation at the start indicating elastic deformation. During this phase, the interface resists the applied deformation without any significant atomic rearrangement or crack propagation. The peak load represents the onset of crack propagation and atomic bond breaking. It can be observed from the figure that with increase in notch size, the peak load is decreasing, i.e. models with larger cracks are more susceptable to failure than those with smaller cracks. After the peak load, the force decreases as the interface experiences plastic deformation, atomic separation, and crack propagation. The decline is steeper for larger notches due to their reduced ability to resist further deformation. The curves show a softening trend in all the cases similar to the fracture behavior of large scale specimens. It should be noted that the continous bonding and de-bonding of the atoms due to reactive force-field results in the spikes observed in the curves. The post-peak decline in smaller notch (11 x 8 Å) is more gradual implying the presence of crack bridging and energy dissipation mechanisms. The sharp decline in 20 x 8 Å specimen after the peak load suggests rapid crack propagation with minimal energy dissipation. These observations are in concordance with the visual inspection of the fracture processes using MD simulations. Thus, highlighting the role of MD simulations in understanding the fundamental mechanisms governing fracture behavior of concrete-like materials.

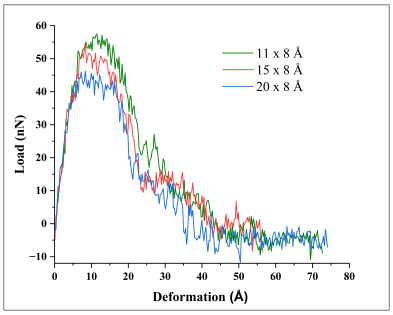


Figure 5: Load-deformation curves for varying notch sizes.

For analysing the response of the interface model with initial notch in CSH and silica, the load-deformation curve is plotted along with the interface-notched specimen as shown in Fig. 6. All curves exhibit a similar initial linear region, corresponding to the elastic deformation phase, where the load increases proportionally with deformation. The slope for the silica notch is steeper indicating higher stiffness and resistance to deformation due to its greater structural rigidity compared to the CSH layer. The lower peak load and early failure in CSH suggests that the CSH layer is more prone to fracture as compared to interface silica cracked specimens. The silica-notch model exhibits sustained load-bearing capability even after reaching peak load due to crack bridging and the high strength of Si-O-Si bonds in the silica layer. Hence, the fracture tends to propagate toward the weaker CSH layer as seen from visual inspection also. These findings offer a deeper understanding of the influence of microcracks and voids in various regions of concrete on the overall behavior of large-scale structures.

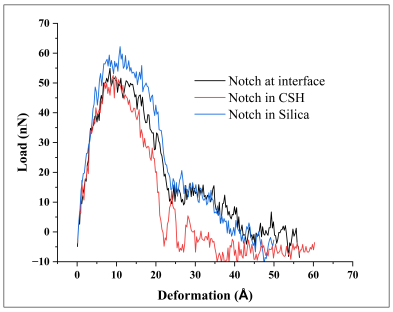


Figure 6: Load-deformation curves for different notch orientation.

The effect of notch size and orientation on the fracture behavior of the CSH-silica interface is further analysed by estimating the mechanical and fracture parameters. The Young's modulus (E) for all the specimens is determined from the slope of elastic portion of the stress-strain curve [17]. The corresponding values are reported in Table 1. It can be seen from the table that with increase in notch size, the Young's modulus is decreasing, indicating a reduction in material stiffness with larger microvoids. The presence of notch in CSH has no effect on the Young's modulus as it's value is comparable to the interface cracked model with same notch length. However, the stiffness of silica notched model is found to be largest among all other models attributing to the stronger covalent bonds in silica.

Table 1: Estimation of mechanical and fracture parameters

Notch Specification	Young's Modulus (GPa)	Fracture Energy (J/m^2)	Fracture Toughness $(MPa\sqrt{m})$
11 x 8 Å	34.46	1.17	0.21
15 x 8 Å	33.72	0.92	0.18
20 x 8 Å	31.61	0.75	0.16
CSH-notched	33.20	0.67	0.15
Silica-notched	44.64	1.05	0.22

Furthermore, critical energy release rate (fracture energy) during the tension simulation is analysed and fracture toughness is calculated for all the models. The fracture energy (G_c) signifies the fracture resistance of the material and is calculated as [18]:

$$G_c = \frac{E_{input}}{\Delta A} = \frac{L_x \cdot L_y \cdot L_y}{\Delta A} \int_0^{\epsilon_0} \sigma d\epsilon \qquad (2)$$

where E_{input} is the input energy of the model. ΔA is the difference between the initial and fractured surface area following the complete rupture and is calculated using Construct Surface Mesh module in the OVITO [16]. L_x, L_y, and L_z are initial dimensions of the simulation box along the x, y, and z directions. At a given moment, σ and ϵ denote the stress and strain of the model in the loading direction, and ϵ_0 is the strain at which the stress in the model reaches zero for the first time after fracture. Fracture toughness (K_{IC}) is then calculated by Irwin's formula [19]:

$$G_c = \frac{1-\nu^2}{E} K_{IC}^2 \qquad (3)$$

where ν is the Poisson's ratio which is taken as 0.3 as per Pellenq et al. [1]. The calculated values of fracture energy and toughness are reported in Table 1. It can be inferred that the fracture energy decreases as the notch size increases, which is in line with the observations reported by Cao et al. [17]. The decrease in fracture energy is upto 21% and 35% for the increase in notch length to 15 Å and 20 Å, respectively. The fracture toughness also follows the decreasing trend for increasing notch size. It is worth noting that while the Young's modulus remains comparable for notch orientations at the interface and within the CSH gel for the 15 x 8 Å crack length, the fracture energy is lower for the CSH-notched model, explaining its earlier rupture. The silica notched model exhibits the fracture energy and toughness comparable to that of interface model with smaller crack. This corroborates the fact that the silica notched model show cracking behavior similar to un-notched or small crack specimens. Hence, it can be concluded that larger notch size and unfavourable orientations lead to accelerated crack propagation and reduced fracture resistance.

4 CONCLUSIONS

This study investigates the effect of notch size and orientation on the fracture behavior of the CSH-silica interface using molecular dynamics simulations. It has been observed that larger notches lead to earlier failure and reduced stiffness, with up to 35% reduction in fracture energy for a 20 Å notch. The smaller notches exhibit higher energy dissipation and fracture toughening through atomic chain bridging. The orientation also plays a significant role in the cracking behavior of the interface. It was revealed that notches in CSH promote rapid crack propagation due to disrupted interlayer hydrogen bonds. In contrast, silica-notched models initially resist fracture owing to strong Si-O-Si bonds but eventually experience cracking near the interface. Mechanical analysis shows a decrease in Young's modulus with larger notches, while silica-notched models exhibit the highest stiffness and sustained load-bearing capability. The findings highlight that larger notch sizes and unfavorable orientations accelerate crack growth and reduce fracture resistance, offering insights into the role of microstructural defects in concrete's overall behavior.

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