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PROCEEDINGS

Atomic-Scale Mechanical Enhancement in Fiber-Reinforced Concrete: A Molecular Dynamics Comparison of Glass and Basalt Fibers

Rui Yang*

China Three Gorges University, Yichang, 443002, China

*Corresponding Author: Rui Yang. Email: y2680295693@163.com

ABSTRACT

This study employs molecular dynamics (MD) simulations to comparatively investigate the mechanical enhancement mechanisms of glass fiber-reinforced concrete (GFRC) and basalt fiber-reinforced concrete (BFRC). Amorphous models of glass fiber (GF) and basalt fiber (BF), along with calcium silicate hydrate (C-S-H), were constructed using the ClayFF force field in LAMMPS. The interfacial transition zone (ITZ), atomic bonding characteristics, stress distribution, and tensile failure processes were systematically analyzed. Key findings reveal that BF exhibits a denser atomic network structure with higher coordination numbers, driven by the bridging role of Fe and Mg atoms. BFRC demonstrates significantly stronger interfacial adhesion, with interfacial binding energy and work of adhesion 1.22 times higher than those of GFRC. Uniaxial tensile simulations highlight BFRC's superior tensile strength and toughness, characterized by delayed microcrack initiation, slower crack propagation, and efficient stress redistribution through interfacial interactions. Fracture in BFRC occurs near the fiber-matrix interface, minimizing damage to the C-S-H matrix, whereas GFRC fails within the calcium-water layer of C-S-H. These results underscore the critical role of atomic-level interactions and interfacial stress transfer in enhancing mechanical performance, providing molecular insights for designing advanced fiber-reinforced concrete materials.

KEYWORDS

Glass fiber; basalt fiber; concrete; mechanical enhancement; molecular dynamics; interfacial transition zone

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