

PROCEEDINGS

Interface Degradation in Basalt Fiber-Reinforced Cementitious Composites Under Hygrothermal Conditions: A Molecular Dynamics Study

Rui Yang^{1,*}¹China Three Gorges University, Yichang, 443002, China

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

ABSTRACT

The long-term performance of basalt fiber-reinforced cementitious composites (BFRCC) is critically compromised due to fiber-matrix interfacial degradation under hygrothermal environments, however, the underlying micro-mechanisms governing this degradation remain poorly understood. In this study, molecular dynamics (MD) simulations are conducted to systematically investigate the interfacial structure, interaction mechanisms, and mechanical properties of basalt fiber (BF)/calcium silicate hydrate (C-S-H) composites under hygrothermal conditions, with interfacial water layer thicknesses ranging from 1 Å to 4 Å and temperatures from 20°C to 60°C. Results show that as the water layer thickness increases, the dominant form of interfacial water transitions sequentially from adsorbed water to confined water and finally to free water, with molecular mobility significantly enhanced by elevated temperature. The hydrogen bond network evolves from cross-interface bridging bonds into an intra-aqueous network dominated by weak water-water interactions, leading to a marked reduction in interfacial stress transfer capability. The interfacial binding energy decreases by 94.64%, reflecting a fundamental shift from direct polar surface coupling between BF and C-S-H to a weak water-water hydrogen bond-mediated bonding mechanism. Under uniaxial tensile loading, the peak tensile force and fracture energy decrease by 81.69% and 90.45%, respectively, with the fracture mode transitioning from bridging-chain-mediated failure to rapid debonding of the free water layer. These findings provide atomistic-scale insights into the hygrothermal degradation mechanisms of BFRCC, offering a theoretical basis for optimizing fiber-matrix interface design and enhancing long-term durability in harsh service environments.

KEYWORDS

Basalt fiber-reinforced cementitious composites; calcium silicate hydrate; hygrothermal environment; interfacial properties; molecular dynamics simulation

Funding Statement: The author receives no specific funding for this study.**Conflicts of Interest:** The author declares no conflicts of interest to report regarding the present study.

Copyright © 2026 The Author(s). Published by Tech Science Press.

This work is licensed under a Creative Commons Attribution 4.0 International License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.