Molecular Dynamics Investigation of Steel Nanofiber Mechanics with Passive Coatings: A Core–Shell Modeling Approach

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Abstract

Both hydroxylation and surface oxidation have primary roles in steel nanofiber mechanical properties. The chemical reactions, resulting from contact with water vapor, oxygen, and corrosive environments, lead to the alteration of the atomic composition of the surface of the nanofiber and form layers whose properties are different from pure steel. In the present paper, a study of the effects of these processes on compressive and tensile mechanical properties of steel nanofibers through molecular dynamics methods using the reactive force field potential (ReaxFF) and core-shell modeling approach has been discussed. Simulations are performed using LAMMPS software with a quasi-static incremental loading scheme to minimize dynamic stresses. It has been found that higher oxide layer thickness reduces Young's modulus, yield stress, and ultimate strength of the nanofibers. Most notably, a 20% oxide layer thickening can reduce Young's modulus by up to 40% and yield stress by up to 34%. Hydroxylation causes these values to become even lower due to its ability to create weaker and less stable bonds. The analysis of the stress-strain curve indicates that the layers of oxide and hydroxide facilitate stress concentration and increase material failure. Experimental evidence corroborates the simulation results and demonstrates the high accuracy of the numerical model. The findings of the present study indicate that when steel nanofibers are exposed to the alkaline condition of concrete, widespread yield stress and Young's modulus reduction will be witnessed, which should be accounted for in the application of such components.

Keywords

steel nanofibers, surface oxidation & hydroxylation, molecular dynamics, mechanical behaviour, numerical simulation.

1. Introduction

Reinforced concrete is a composite of hardened cement and mineral aggregates, which is further strengthened by a variety of fibers. It is one of the most widely used building materials and is employed extensively in civil projects such as roads, load-bearing structures, and airport runways. In modern construction, additives and reinforcing fibers play a key role in improving concrete quality and performance. These additives can be used at various scales, and besides enhancing mechanical properties, they help reduce weight and provide lighter materials to engineers. Research has shown that adding nanometer-scale particles and steel fibers in proportions of 1–5 % by weight can increase tensile strength by up to 100 %, flexural strength by 150–200 %, and compressive strength by 10–25 % [1]. When uniformly distributed in the concrete matrix, they allow better exploitation of high-strength concrete [2]. In fine steel fibers, the oxide and hydroxide layers that form on the steel surface through natural oxidation and hydroxylation in the alkaline concrete environment play a crucial role in determining the mechanical behaviour of these materials. Although these layers act as protective coatings against corrosion, their effects on mechanical properties, especially at the nanoscale, require detailed study [3].

The present research investigates how oxidation and hydroxylation influence the tensile and compressive behaviour of steel nanofibers using molecular dynamics, the ReaxFF reactive force field, and a core–shell model. This work quantitatively relates oxide-layer thickness to reductions in mechanical properties, filling a gap in the literature. It examines three oxide-layer thickness levels and compares the effects of oxidation and hydroxylation on the mechanical response of steel nanofibers under tensile and compressive loading.

2. Modelling Details

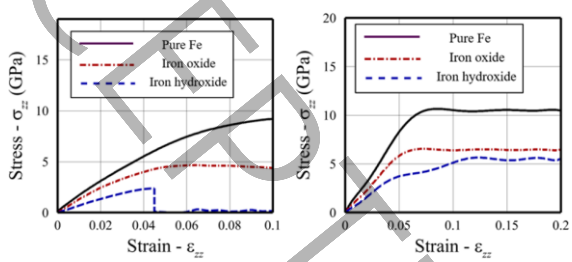
In MD simulations, atomic interactions are modelled using interatomic potential. The ReaxFF reactive force field [4] is chosen for this study because it accurately captures bond formation and breakage, as well as the diverse bonding environments in metallic, ionic and covalent systems. The initial atomic configurations for pure iron, Fe_2O_3 and FeOOH were constructed from the crystal structures. The iron nanofibre was first built as a BCC lattice, and an oxide or hydroxide shell was grown around it using a core–shell scheme.

The system was first equilibrated in an NPT ensemble at 300 K and 1 atm for 100 ps to minimize residual stresses. Then an NVT run of 100 ps was performed to reach thermal equilibrium. The time step was set to 1 fs, and all simulations were carried out in LAMMPS. Tensile and compressive loading were applied quasi-statically by incrementally deforming the simulation cell in the axial direction. Each deformation step consisted of a 6 ps strain application followed by a 12 ps relaxation (step-wise loading). This procedure suppresses dynamic stresses that would otherwise arise from the high strain rate typical of MD.

3. Results and Discussion

After equilibration, radial distribution functions (RDFs) were computed for Fe–O, O–O, Fe–H, and H–H pairs. In the Fe_2O_3 structure, the Fe–O peak at ~2 Å indicates strong covalent/ionic bonds. In FeOOH, the Fe–O peak shifts slightly and is accompanied by a Fe–H peak (~1.8 Å), showing the presence of hydroxyl groups. The H–H peak (~1.5 Å) confirms hydrogen clustering. These structural features explain the reduced mechanical performance of hydroxylated fibers. Stress–strain curves for pure iron, oxide-coated, and hydroxide-coated nanofibers are shown in Fig. 1. Pure iron exhibits a high Young's modulus (~138 GPa) and ultimate tensile strength (~7.4 GPa).

Oxide coating reduces modulus by 5–16 % and strength by 20–30 % depending on thickness. Hydroxide coating leads to larger reductions, with modulus dropping to ~4.5 GPa for 20 % thickness of Oxide coating.



(a) (b)

Fig 1. Stress-strain graphs of atomistic RVE under (a) tensile and (b) compression loading.

Increasing oxide-layer thickness from 0 to 20 % leads to a roughly linear decrease in both Young's modulus and ultimate strength. Hydroxylation amplifies this trend. The presence of the oxide/hydroxide shell concentrates stress at the core–shell interface, promoting crack initiation and rapid failure. The results underscore that fine steel nanofibers will experience substantial strength loss when exposed to the alkaline pore water of concrete. In particular, the hydroxy-layer formation, which is promoted by high moisture content, exacerbates the degradation. Therefore, in concrete design, surface treatments (e.g., protective coatings, alloying, or controlled passivation) are essential to preserve the mechanical advantages of steel nanofibers.

4. Conclusion

The study demonstrates that surface oxidation and hydroxylation substantially degrade the mechanical properties of steel nanofibers. An oxide layer thickness of 20 % reduces Young's modulus by ~95 % and ultimate stress by ~31 %. Hydroxylation further lowers modulus to ~4.5 GPa and ultimate stress by ~20 %. These effects are more pronounced under compression. The core–shell MD model with ReaxFF accurately captures these trends and agrees with experimental data. Design of reinforced concrete incorporating steel nanofibers must account for the loss of strength due to oxidation/hydroxylation, especially in the alkaline environment of concrete.

References

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