Uncertainty-Aware Modeling of Structural Reliability in Energy Systems

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Introduction

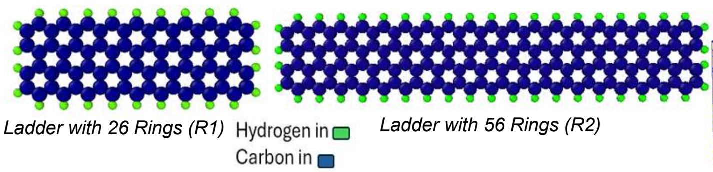
Carbon fiber (CF) was chosen as the material of focus for this project due to its high modulus of elasticity (200–600 GPa), low density (1.7–2.0 g/cm³), and excellent thermal resistance. These properties make CF widely used in industries such as defense, aerospace, and energy, where lightweight, high-strength materials are essential.

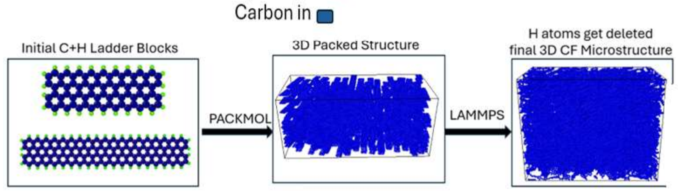
Previous studies have provided important Hugoniot observables but have not fully explained how the graphite microstructure evolves during shock compression. Molecular dynamics (MD) simulations address this limitation by tracking the motion of individual atoms under dynamic loading. Most MD studies have focused on carbonization, ladder formation, and ring statistics, leaving the shock response of fully constructed three-dimensional carbon fiber microstructures largely unexplored.

The goal of this project is to build upon the work of Afia Kona and Alireza Tabarraei by constructing and analyzing an R1R2-Z10 carbon fiber microstructure using molecular dynamics simulations. This study aims to further investigate the shock response of three-dimensional carbon fiber microstructures.

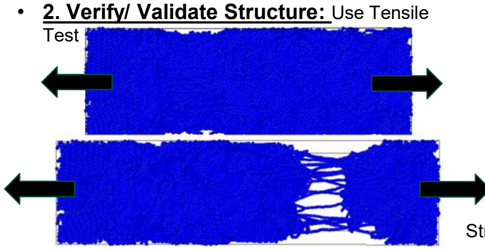
Method

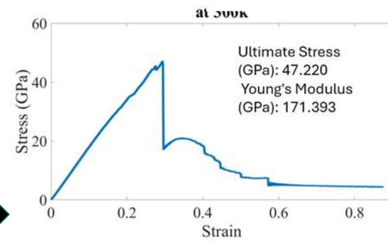
- **1. R1R2-Z10 Creation:** C+H ladder building blocks are packed with PACKMOL, then equilibrated in LAMMPS and dehydrogenated to yield the final 3D carbon fiber microstructure (10 degrees in Z direction is ladder angle)





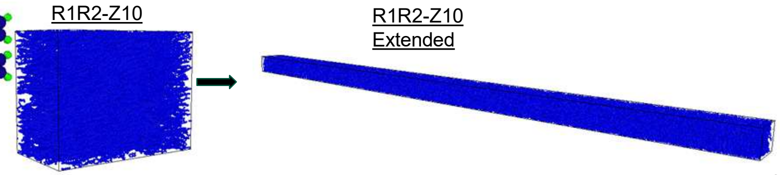
- **2. Verify/ Validate Structure:** Use Tensile Test



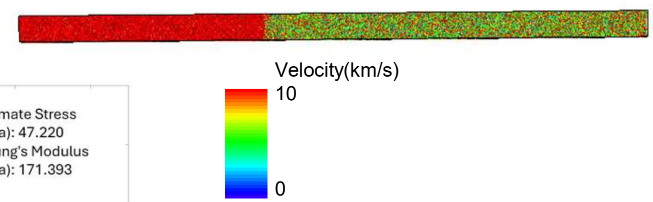


Structure Behaves as Expected for Carbon Fiber at 300K

3. Shock: Shock loading is applied along the z-direction of the CF microstructure. To accommodate this configuration, the equilibrated structures are reoriented such that their longest dimension aligns with the shock propagation direction. Then the Structure is Equilibrated

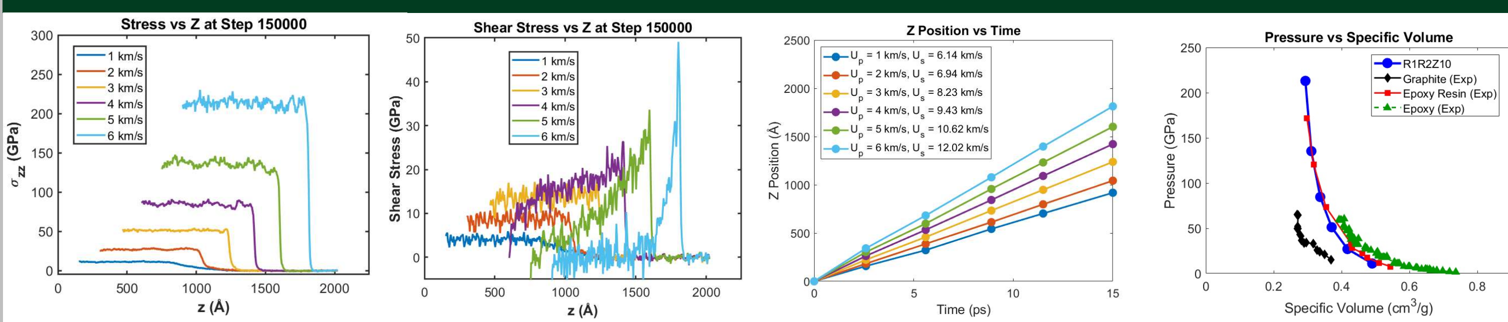


Next, Piston-driven shock simulations are employed to investigate the dynamic response of equilibrated carbon fiber (CF) microstructures under extreme loading conditions.



Process Is Repeated for six different shock velocities, V= 1-6 km/s

Results



Results: The results show that the carbon fiber microstructure responds consistently to increasing shock intensity. The stress and shear stress profiles show the formation of a shock front and increasing deformation at higher piston velocities. The shock-front position varies linearly with time, allowing the shock velocity (U_s) to be determined. The pressure–specific volume results also follow the expected Hugoniot trend, showing increased pressure with greater compression. Overall, the simulations demonstrate realistic shock propagation and dynamic compression behavior in the R1R2-Z10 carbon fiber microstructure.

Conclusions

This project successfully constructed and analyzed an R1R2-Z10 carbon fiber microstructure using molecular dynamics simulations. The results showed that the structure exhibits realistic shock propagation and follows expected Hugoniot behavior under increasing piston velocities. Overall, this work provides a better understanding of the shock response of three-dimensional carbon fiber microstructures and serves as a foundation for future studies on their behavior under extreme loading conditions.

References

Kona, A. A., Ramaprabhu, P., & Tabarraei, A. (2026). *Shock response of carbon fiber microstructure using molecular dynamics simulations*. Preprint