

Postdoctoral Researcher openings at the University of Delaware - Center for Composite Materials

The University of Delaware Center for Composite Materials (UD-CCM) is an internationally recognized center of excellence for interdisciplinary research, education, and technology transfer providing world-class research to both industry and government sponsors.

In the Army Research Laboratory sponsored 'Materials in Extreme Dynamic Environments (MEDE)' program, we developed a molecular dynamics-based "Materials-by-Design (MbD)" framework to design glass fiber-epoxy composite interphase. Using reactive molecular dynamics (MD) simulation with ReaxFF, we studied fiber-matrix interphase and its constituents - glass fibers, epoxy resin, sizing to understand the processing-structure-properties relationship, deformation and damage mechanisms. Using that MbD framework, we developed strain-rate dependent mixed-mode traction law to bridge the length scale (nano to micro to meso) to model composite structures at a larger length scale. Optimizing the complex interphase structure considering wide range of resin and sizing chemistry, and fiber-sizing-resin interactions is beyond simple intuition guided materials selection and simulations. Advances in artificial intelligence and machine learning have given a new opportunity to leverage computational power to explore and optimize the properties of materials. As an extension of this MEDE program, we intend to build upon the existing atomistic modeling approach wrapped in physics informed machine learning (PIML) to discover new mechanisms and improved properties for glass fiber-epoxy composite interphase. We are seeking postdoctoral researchers to develop the machine learning framework for glass fiber-matrix interphase considering wide range of resins and sizing chemistry; variability in interphase topology – monolayer versus multi-layer sizing; and pressure/temp/strain rate effects. Input data for the machine learning should be generated from all-atom and/or coarse-grain (CG) MD simulations.

Major Responsibilities

- Develop physics informed machine learning (PIML) framework to optimize glass fiber-matrix interphase.
- Molecular dynamics (MD) based computational modeling and analyses.
- Develop structure-property data set (especially interphase traction laws) for interphase at ambient as well as extreme conditions (high temperature and high strain rates) to use them in PIML.
- Conduct coarse-grain (CG) modeling for input data generation for PIML if necessary, to reduce computation cost.
- Present work including theory, approach, results, and conclusions at ARL review meetings; report findings via government publications (technical reports), peer-reviewed publications, and conference presentations.
- Perform miscellaneous job-related duties as assigned.

Qualifications

- Ph.D. in Mechanical Engineering, Materials Science and Engineering, or relevant disciplines.
- Strong background in machine learning with conventional and advanced techniques (CNN, VAE, UNet, Bayesian Optimization etc.).
- Experience in all-atom MD modeling using advanced tools preferably with LAMMPS using reactive (ReaxFF) and non-reactive force fields.
- Experience in coarse-grain modeling using advanced tools preferably with LAMMPS.
- Experience in coarse-grain force field development.
- Expert in parallel computing and utilizing advanced computer simulation and visualization tools (LAMMPS, Ovito, VMD etc.).
- Proficient in programming languages (Matlab, Python etc.) to develop scripts for data analysis.
- Strong background in composite mechanics and interphase.
- Ability to write high quality journal papers by planning and conducting systematic analysis and summarizing and organizing simulations data.
- Demonstrates an understanding and consideration of the differing needs and concerns of individuals with varying identities, cultures and backgrounds.
- Committed to fostering a workplace culture of belonging, where diversity is celebrated, and equity is a core value.

Notice of Non-Discrimination, Equal Opportunity, and Affirmative Action

The University of Delaware does not discriminate against any person on the basis of race, color, national origin, sex, gender identity or expression, sexual orientation, genetic information, marital status, disability, religion, age, veteran status or any other characteristic protected by applicable law in its employment, educational programs and activities, admissions policies, and scholarship and loan programs as required by Title IX of the Educational Amendments of 1972, the Americans with Disabilities Act of 1990, Section 504 of the Rehabilitation Act of 1973, Title VII of the Civil Rights Act of 1964, and other applicable statutes and University policies. The University of Delaware also prohibits unlawful harassment including sexual harassment and sexual violence.

To apply, please send a cover letter, full resume and three recommendations to: hamed@udel.edu