Graphite-templated Pyrolysis Modeling of Phenolic Resins for Enhanced Carbon-Carbon Composites in Hypersonic Applications

About AFRL:

Air Force Research Laboratory (AFRL) is a research organization of United States Air Force under Department of Defense. It consists of over 9 directorate spread over continental United States and Hawaii. AFRL's mission is to lead the discovery, development, and integration of aerospace warfighting technologies, planning and executing the Air Force science and technology program, and providing warfighting capabilities to United States air, space, and cyberspace forces. It strives to advance the capabilities of both Air Force and Space Force (under the umbrella of One Lab: Two Services) by conducting innovative research, development, and testing across various scientific and technological disciplines. This mission encompasses enhancing war-fighting effectiveness, ensuring national security, and driving advancements in aerospace capabilities to meet the evolving challenges of the future.

RESEARCH LOCATION: Wright-Patterson AFB, OH

PROJECT DESCRIPTION:

Using atomistic molecular dynamics simulations, this proposal will model the pyrolysis of phenolic resins near graphic planes and surfaces (mimicking surfaces of carbon fiber). All the simulations will be performed using DSRC resources. The effort will provide needed insights on the role carbon-fiber play in modulating the graphitic content and other micro-structural features (porosity, ratio to sp2/sp3 atoms), which have significant impact on thermal (thermal conductivity, thermal stability, thermal protection) and mechanical (modulus, structural integrity) properties for hypersonic applications.

AFRL has recently formulated a novel framework to model the pyrolysis of amorphous phenolic resins using the ReaxFF force field. In this project, the plan is to expand the framework by utilizing a combination of much faster Interface-Force Field (IFF) with ReaxFF and model the graphite-templated pyrolysis of phenolic resins to understand how phenolic resins char near carbon-fibers surfaces via MD simulations via LAMMPS.

The plan is to investigate the differences of morphological features (graphitic content, porosity, ratio of aromatic and aliphatic carbons) of charred resin, near and away from the interface. Such study will provide much-needed insights in optimizing the processing conditions for high-thermally conductive carbon-carbon composites for hypersonic applications. The project plan will involve:

- Build composite systems of graphite-phenolic resin interface, including phenolic crosslinking via IFF
- Crosslink phenolic resins using faster IFF force-field
- Model the pyrolysis of the crosslinked resin using ReaXFF
- Investigate the differences in microstructural feature

The intern will be involved in multiple activities for their technical and professional development. Intern activities will include systematically working on the simulations as highlighted in the project plan that will involve building the composite systems, crosslinking phenolic resins at the interface, model the pyrolysis, and investigate the pyrolyzed char characteristics as a function of different microstructural features. The intern will also attend weekly research meetings of ceramics and will be involved in participating in other ceramic and carbon/carbon research activities based on their availability. The intern will also present their summer work as a presentation in research team meetings and as a part of RX-wide poster session towards the end of the internship. These activities will help in the professional growth of the intern, not only from the perspective of communication and presentation skills, but also from the perspective of how to present the research to world-class experts of diverse technical areas. It is anticipated the AFRL-DRSC will arrange a tour of HPC facilities for the intern to appreciate DoD world-class facilities. AFRL-RX hosts over 150 summer students as part of different programs. So, this lively setting will also help intern interact with other interns, learn about their work and broader their professional knowledge.

ANTICIPATED START DATE:

May 2024 – Exact start dates will be determined at the time of selection and in coordination with the selected candidate.

QUALIFICATIONS:

The ideal candidate should be knowledgeable in LAMMPS Molecular Dynamics package and have proficiency in pre- (how to write input scripts and create new systems) and post (analyze LAMMPS results) processing of data for before and after the simulations. Some knowledge of how to utilize high performance computing resources will also help accelerate the productivity of the project. The candidate should also have good technical, communication, and inter-personal skills to interact with other AFRL researchers, doesn't hesitate to ask critical questions and follow up. Prior background with modeling carbon based polymeric systems or carbon-carbon composites will be useful.

ACADEMIC LEVEL:

Degree received within the last 60 months or currently pursuing:

- Master’s
- Doctoral

DISCIPLINE NEEDED:

- Chemistry and Materials Sciences
- Computer, Information, and Data Sciences
- Engineering
- Science & Engineering-related