NASA EPSCoR
Research Performance Progress Report (RPPR)
Seed Award

I. Collaborating Organizations

A. Academic Collaborators *(do not include names of minors)*

Name	Academic Affiliation	RID Project Role	Nearest person month worked	Contribution to Project	Funding Support
Dr. Nuwan Dewapriya	University of Delaware, Center for Composite Materials	Principal Investigator	1	Conducted molecular dynamics modeling, data analysis, manuscript preparation, and coordination with NASA collaborators.	NASA EPSCoR
Dr. John W. Gillespie, Jr.	University of Delaware, Center for Composite Materials	Co-Investigator	0	Technical guidance and review of PI's research activities.	N/A

B. NASA Collaborators

Name	Title	NASA Center	Nature of the Collaboration
Dr. Evan J. Pineda	Research Aerospace Engineer	Glenn Research Center	Providing guidance on research direction and review of modeling results.
Dr. Brett A. Bednarcyk	Materials Research Engineer	Glenn Research Center	Providing technical inputs and review of results.

C. Industry Collaborators

Name	Title	Industry/Company Name	Nature of the Collaboration

D. New non-EPSCoR grants

Funding Entity	Award Name	Value of New Grant
Department of Defense	DARPA'S Advanced Research Concepts	$265,513

E. Other Organizations Involved as Partners

Organization	Nature of the Partnership	Benefit of the Partnership

II. Products

A. List Journal publications – Please only list papers that have been published. **Please do not remove the table; or alter columns, add additional rows as required.**

Date Published	Published Paper (APA format)

B. List Conference Papers – Please only list papers that are included in conference proceeding. **Please do not remove the table; or alter columns, add additional rows as required.**

Conference Date	Conference Paper (APA format)

C. List Conference Presentation – Please list conference presentation. **Please do not remove the table; or alter columns, add additional rows as required.**

Conference Date	Presentation Topic (APA format)

D. List Books and/or other Publications – Please include explanations, help us to learn about your accomplishments. **Please do not remove the table; or alter columns, add additional rows as required.**

Date	Explanations (APA format -Book, Newspaper Op-Ed, …)

E. List talk/presentation/event/outreach activity – Please include explanations, help us to learn about your accomplishments. **Please do not remove the table; or alter columns, add additional rows as required.**

Date	List talk/presentation/event/outreach activity (APA format if applicable)

F. List of new or updated Website(s) or other Internet site(s). **Please do not remove the table; or alter columns, add additional rows as required.**

URL	Short description of purpose of site

G. Technology/Technique – **Please do not remove the table; or alter columns, add additional rows as required.**

Technology/Technique	Short description of technologies or techniques

H. List patent – Please include Patent Number/Patent Title/ Patent Abstract (or link to it). **Please do not remove the table; or alter columns, add additional rows as required.**

Date Patent Issued	Patent Number/Patent Title/ Patent Abstract (or link to it)

I. List Inventions – Please include Invention Title, List of Inventor(s) and Description. **Please do not remove the table; or alter columns, add additional rows as required.**

Invention Title	List Inventor(s)	Invention Description

J. List Licenses – Please include license issued, Invention Title, List of Inventor(s) and Description. **Please do not remove the table; or alter columns, add additional rows as required.**

Date License Issued	License Assignees	License Title

K. List New/Revised Courses – Please include new/revised courses. **Please do not remove the table; or alter columns, add additional rows as required.**

Course Number	Course Name/Title	Offering Institution

L. Others: List Databases, Physical collections, Audio or video products, Software or NetWare, Models, Instruments or equipment, Data & Research Material (e.g., cell lines, DNA probes, animal models) related to your EPSCoR research. **Please do not remove the table; or alter columns, add additional rows as required.**

Accomplishments title	Short Description of accomplishments

III. Changes/Problems

A. Actual or anticipated problems or delays and actions or plans to resolve them

There are no actual or anticipated problems or delays at this time. The work is progressing as planned, and we are on track to complete a journal manuscript by the end of the seed award period. The results generated under this grant will also serve as the foundation for preparing a full proposal.

B. Changes that have a significant impact on expenditures

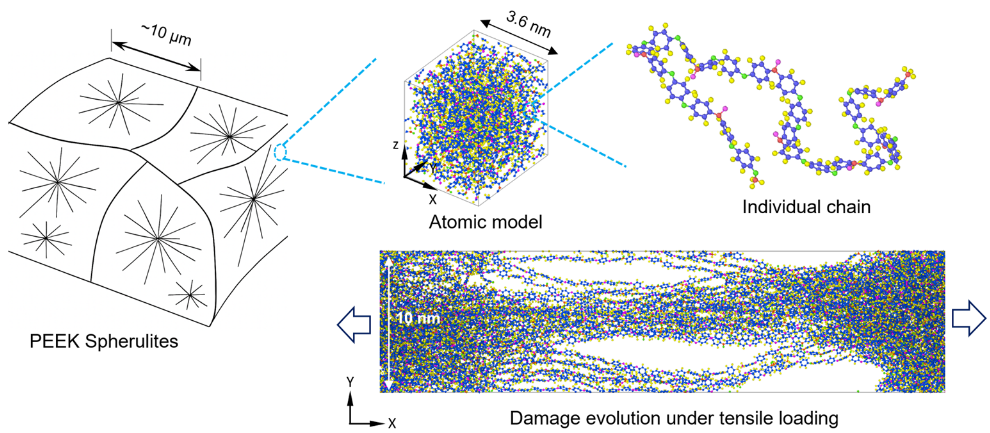
An undergraduate research assistant with the required background was not identified during the previous summer period. As a result, planned undergraduate support funds were not expended during that time. This did not impact the technical progress or timeline of the project.

IV. Impact

Seeing Inside Advanced Polymers: How Molecular Simulations Enable Safer, Lighter Aerospace Structures

High-performance thermoplastic polymers such as poly(ether ether ketone) (PEEK) are increasingly used in aerospace structures because they offer high specific strength and stiffness, along with excellent thermal and damage tolerance. However, predicting how these materials deform and accumulate damage under extreme mechanical loading remains a major challenge, since their performance is governed by molecular-scale processes that cannot be directly observed in experiments.

This NASA EPSCoR seed project bridges length scales by connecting real polymer microstructures to molecular-level simulations and, ultimately, to material failure. At the largest scale, PEEK consists of micron-sized spherulitic structures that control stiffness and strength. Zooming in, atomistic simulation models capture thousands of polymer chains interacting within nanoscale volumes, while individual chains reveal how molecular segments stretch and reorient under load. These simulations make it possible to directly observe how molecular deformation evolves into localized damage and loss of load-bearing capacity under tensile loading.



Multiscale simulations link molecular-scale polymer behavior to deformation and damage in advanced thermoplastic materials, enabling predictive design of lightweight aerospace structures

By integrating molecular dynamics simulations with multiscale modeling tools, the project quantifies how temperature and loading rate influence stiffness, strength, and damage evolution in amorphous regions of thermoplastic materials. The resulting physics-based mechanical properties can be incorporated into NASA's Multiscale Analysis Tool (NASMAT), enabling more accurate predictions of structural performance while reducing reliance on costly experimental testing.

Beyond its immediate technical outcomes, this work strengthens NASA–university collaboration, advances computational research infrastructure, and trains the next generation of aerospace engineers in predictive materials modeling. Together, these advances lay the groundwork for future NASA efforts to design lighter, safer, and more reliable aerospace structures using advanced polymer materials.