Visitor Research Report

Visitor Name:	**Mr. Ananyo Bandyopadhyay** **Michigan Technological University**
Area of Research:	**Multiscale Modeling of the Effects of Physical, Chemical, and Hydrothermal Aging o Failure of Graphite/Epoxy Composites**
Period of Visit:	**August 3, 2009 – August 28, 2009**

Goal:

My goal while visiting NIA for one month was to discuss the details of my PhD project with Dr. Kristopher Wise and Dr. Thomas Clancy and get important suggestions from them. I started working on my research last year and made computational models of epoxy polymer precursors and started forming cross-link bonds in the models. My trip to NIA was mainly to show Dr. Wise and Dr. Clancy the process I have developed for building the models and to get their suggestions about what changes I need to implement in these models to make them more realistic. Through a number of meetings, I learned what parameters I need to monitor and what I need to change in these structures to make them more representative of bulk scale polymer materials. Also, while modeling hydrothermal aging, I will need to put in water molecules with charges in the polymer models and the process of modeling these moisture containing structures was discussed in detail with Dr. Clancy and Dr. Wise.

Strategy:

Before coming to NIA, I had already generated density, volume shrinkage and glass-transition temperature values for my 50% cross-linked models and I was constructing the highest (84%) cross-linked structure. At NIA, I finished building the 84% cross-linked model and studied the same properties for this model. The results were not as encouraging as the 50% cross-linked model but after long discussions with Dr. Wise I identified some of the errors I made while building my model. Dr. Clancy had some other suggestions. My seminar at NIA allowed me to show my work to other researchers in NASA and after the seminar, I had a long discussion with Dr. Jeffrey Hinkley and Dr. Wise about what needs to be done in the future on this project. A number of their suggestions will be implemented in my models.

Accomplishments:

The properties obtained in the 50% cross-linked model were comparable to experimental results but the values were not sufficient to determine if the models had some inherent flaws in them. Each model had 27 cross-linked small polymer systems and each system

had 936 atoms. There were 25272 total atoms in each model. Although the 27 systems were internally cross-linked, I did not form cross-links in between these 27 systems because of the difficulty in modeling cross-links of such large structures. This approximation did not cause any errors in the calculation for the 50% cross-linked model, but in the 84% cross-linked model the error led to the separation of the model into 27 sub-systems at high temperatures, and ultimate disintegration of the polymer system. Thorough analysis of the various parameters led to the following improvements that need to be implemented:-

i. Additional cross-linking in between the 27 systems is required. The Python programming language will be used to simplify the cross-linking process
ii. Electrostatic interactions need to be included to partially balance the huge effect of the repulsive van der Waals interactions
iii. Long simulation times, on the order of 1000 picoseconds, are necessary for getting a good knowledge about molecular relaxation
iv. Plotting of all components of energies against time is required in every simulation
v. For hydrothermal aging, water molecules with charges need to be modeled in the structures.

Future Work:
After incorporating the above mentioned changes in the polymer models, I will run simulations and get the density and glass-transition temperature values for the other cross-linked models. It will be interesting to see what effect cross-linking has on these properties. The next part of the project is to make models with various degrees of moisture in them to simulate the conditions of hydrothermal aging. Effects of this aging on mechanical properties will be studied in detail.

Pending Publications:
At present, there are no pending publications.

Seminar Presented:
A seminar on "Atomistic Modeling of Cross-linked Epoxy Polymers" was presented on 21st of August. This included a demonstration of whatever has been done on this project.