Predictive Modelling of Crosslinked Polymer Networks

Industrial Training Project

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MATERIALS SCIENCE AND ENGINEERING
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With the increased acceptance and usage of Carbon Fibre Reinforced Plastics in the aviation industry, there is a growing need for cheaper and quicker validation methods for composite materials. Molecular dynamics simulations offers a potential method to significantly reduce the time and costs in finding as well as testing new resin systems.

Background

Due to its highly desirable mechanical properties, Carbon Fibre Reinforced Composites continue to be used in greater amounts in the aviation industry. Composite materials make up 25% of the airframe of the Airbus A380 and 50% of the Boeing 787 Dreamliner. However, novel resin systems must be found if there is to be continual improvement of aircraft performance. The current methods of resin formulation and testing are extremely resource intensive and time consuming, especially considering the strict guidelines concerning aviation class materials. Molecular dynamics can be used to simulate epoxy resins at an atomistic level and potentially offers a method to characterise new resin systems in a more timely and cost efficient manner.

Aims

Firstly, this project aims to evaluate the accuracy and robustness of one specific method of modelling epoxy resin systems using molecular dynamics. The project then hopes to find structure-property relationships between molecular structures in the resin monomers and the final bulk and thermal properties of the resin.

Method

In order to determine the accuracy and robustness of our method of modelling resin systems, the thoroughly studied Diglycidyl ether of bisphenol A [DGEBA] epoxy cured with 4,4'-Diaminodiphenyl sulfone [DDS] was modelled. The properties of this resin system such as glass transition temperature, yield strain and density were then interrogated using molecular dynamics and results compared to experimental values in literature. The system was also modelled at various simulation sizes, measured by atom count, to see whether the size of the simulation affected the measured properties.

The DGEBA monomer was then systematically varied (See Figure 1) to exaggerate the effects of specific structures in the monomer. The resin systems modelled with these altered DGEBA monomers were also interrogated to see what effect these changes would have on the bulk and thermal properties of the resin.

Results

Key findings include;

- The thermal and mechanical properties of the simulated DGEBA-DDS system closely reflected experimental values found in the literature
- The error in the simulations reduced with increased simulation size
- Computational cost increased linearly with simulation size
- An increased density of aromatic structures in the polymer gives rise to higher glass transition temperatures whereas an increased density of aliphatic structures gives rise to lower glass transition temperatures
- The resins made with the DGEBA epoxy variants showed similar yield strain to the unaltered DGEBA resin save for the structure with aromatic groups pendent to the backbone of the resin

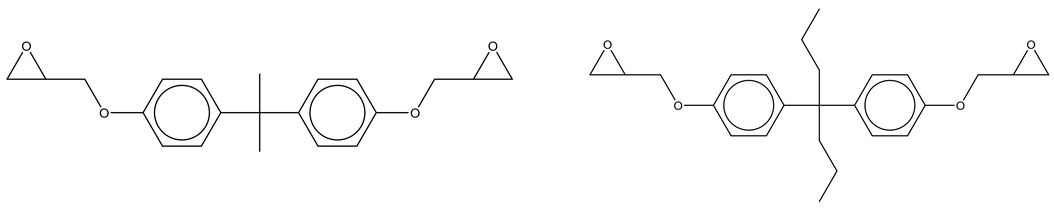

Figure 1: The epoxy monomer DGEBA [left] and an example of how the aliphatic structures were emphasised, in this case pendent to the backbone [right].

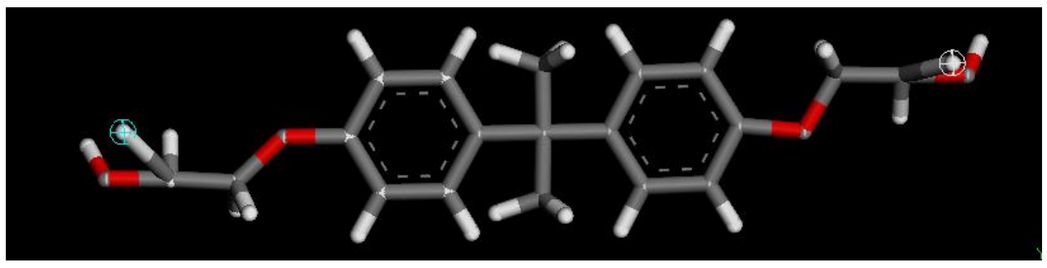

Figure 2: A DGEBA molecule as seen in the Materials Studio Visualiser® with end points marked.

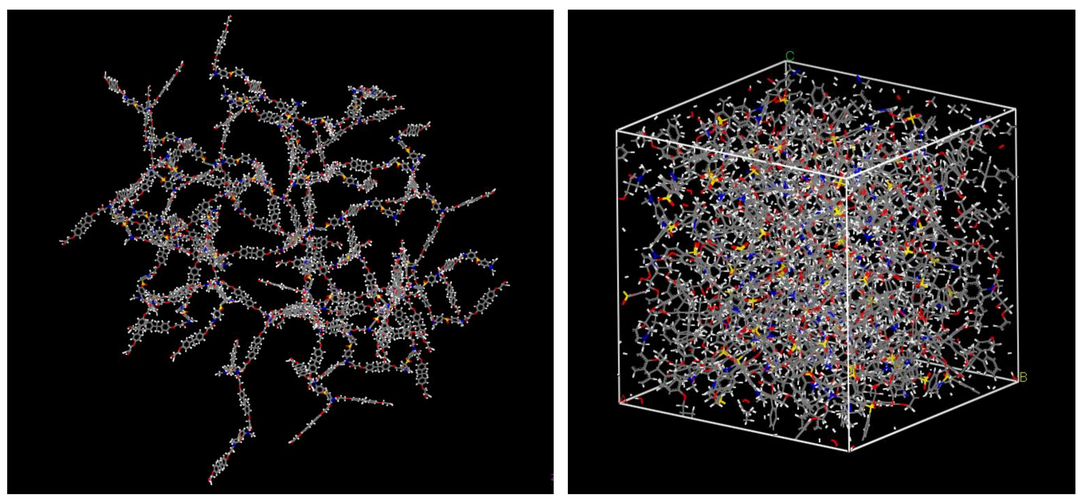

Figure 3: A DGEBA-DDS dendrimer built in Materials Studio [left] and the equilibrated structure at standard temperature and pressure in a unit cell [right] , both as seen in the Materials Studio Visualiser®.

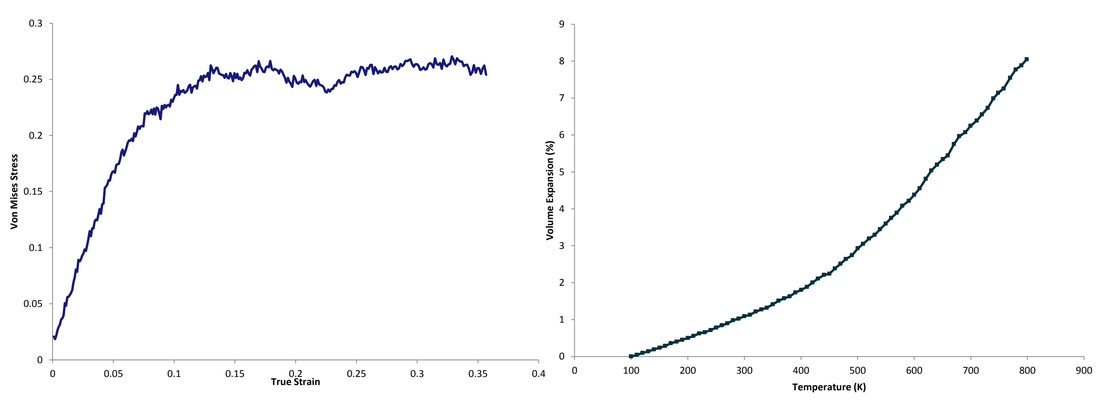

Figure 4: A typical simulated stress strain plot and thermo-mechanical analysis plot of a 30000 atom DGEBA-DDS resin system

Industrial Training Outcomes

- Gained experience and an appreciation for working in a research role
- Developed my understanding of the scientific method and gained exposure to real life limitations a researcher may face
- Improved my presentation and public speaking skills through classes and presenting to my peers
- Was provided very helpful career advice and life stories by current staff on their journey to becoming a research scientist
- Developed connections with science and engineering students from all across Australia
- Attended the Carbon Fibre Future Directions conference in Geelong
- Research to be published in a scientific journal

FOR FURTHER INFORMATION

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