MULTI-SCALE MECHANICAL PROPERTIES OF GRAPHENE-EPOXY NANOCOMPOSITES

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ABSTRACT

Polymer nanocomposites have received great attention in materials research over the past decades. Epoxy, a highly crosslinked thermosetting polymer, is currently used widely in different applications, such as wind turbines, aerospace and automotive industries, and electronics. On the other hand, graphene is an emerging new material, which is finding its way as a promising new alternative nanofiller with novel electrical, thermal, and mechanical properties. Introducing graphene as the second phase to epoxy is known to improve its mechanical properties to a great extent. However, there have been limited studies to investigate mechanics of this type of defective graphene. Understanding the role of defects on mechanical properties of graphene is of great importance for its composite applications as well as the other wide range of applications including thermal interface materials.

This thesis represents a series of experimental evaluations of mechanical properties of graphene. In particular, different levels of defects are introduced using oxygen plasma. State of defectiveness was characterized by Raman spectroscopy, and defective graphene was tested using AFM indentation. It was found that plasma treated graphene preserves its stiffness up to a critical point, and after that it loses the stiffness values. However, it was found that strength was more sensitive to presence of defects.

Computer modeling investigations based on molecular dynamics was also performed to correlate the experimental results on the mechanical properties of defective graphene sheets. Reactive force field (ReaxFF) potential was used to simulate the chemical reactions forming the defects. A verification model of pristine graphene was simulated, and the measured properties were compared with literature. Twinning was found to be the crucial deformation mechanism at high strains and before material's failure. This is also a function of boundary conditions. To simulate plasma treatment of graphene, a sheet of carbon atoms were exposed to oxygen atoms and the defect formation and growth mechanisms were studied. Selected structures were used for mechanical testing. The trend of mod-

ulus and strength compared with experimental observations and good consistency were found. To compare the effects of vacancies and oxygen groups on mechanical properties, artificial structures with different concentrations of vacancies and epoxide groups were generated and tested. Vacancy - oxygen maps of modulus and strength were produced.

Graphene platelets (GPLs) were produced using thermal reduction and used for fabricating graphene epoxy nanocomposites. Dispersion quality of GPLs in epoxy was monitored and found to be optimized at 0.1 wt%. Quasi-static uniaxial tensile tests were performed at different temperatures. Similar tests were performed for fracture toughness. The improvements in yield strength and stiffness of epoxy by GPL is more pronounced at higher temperatures, however, the difference in fracture toughness values diminishes when temperature increases. Nanoindentation is used to probe local mechanical properties in nanocomposite thin films. Creep response of the nanocomposites was also studied at macroscale and different temperatures. GPL reduces creep strain at 55 °C by 30%. Nanoindentation creep tests were also performed using Berkovich and flat punch tips.