

FY 2008 Project Proposal

Project No. AUAD-08

TAILORED SURFACE REACTIVITY OF CARBON NANOTUBES FOR POLYMERIC COMPOSITE APPLICATIONS

Project Team:

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Objective:

New challenges have emerged in the field of new materials, in particular the field of composites, driven by recent technological progress. Dramatic advances in nanotechnology enable the tailoring of the properties at the nano level, allowing for the preparation of light weight composites, suitable for commercial and military applications, with outstanding properties. The proposed research aims to control the nanofiller structure at the nano level, in particular with new methods for surface functionalized carbon nanotubes (CNTs), elucidating the interfaces and interactions between CNTs and different polymeric systems.

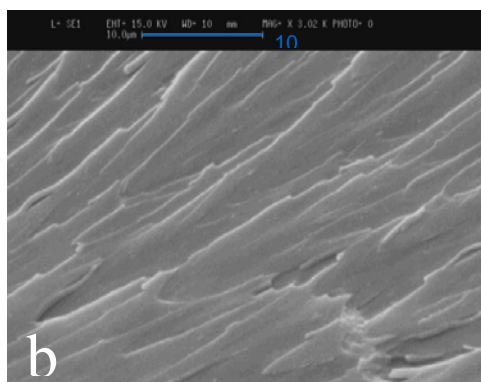
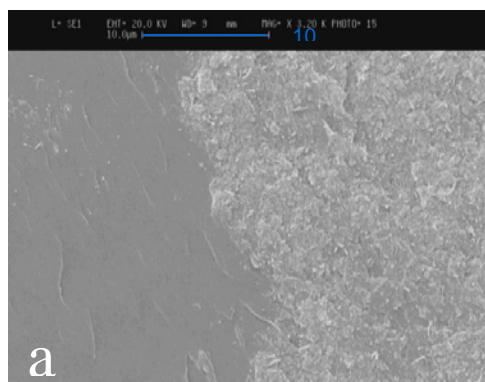
Relevance to the Polymer and Fiber Engineering Department Mission:

The proposed research is based on an interdisciplinary effort that involves polymer surface chemistry, interface manipulation, and advanced nano-microfabrication techniques. The main issues to address during the progress of this proposal are: (i) development of a new generation of functionalized CNTs suitable for a new generation of nanocomposite applications; (ii) achievement of a fundamental understanding of the correlations between the novel nanostructures, the morphology and the physical properties in the final composites. As an additional benefit, these well-correlated structures at different length scales might also provide a solution for the transfer of the novel properties at the nanoscale into a higher length scale. The development of novel composite materials is vital for the U.S. industry to remain competitive. Students will receive training and become skilled in the science and technology of nanomaterials manufacture and functional fibers, certainly relevant to the department mission.

State of the Art:

Carbon nanotubes are believed to be the ultimate low-density high-modulus “fibers”. All of the benefits associated with composite design could thus be implemented on the nanoscale with what are probably the strongest “fibers” available to society. Several works have reported that nanotubes can undergo enormous bending deformation and recover elastically. Recent studies showed that the elastic and shear moduli of individual carbon nanotube ropes are of the order of 1 TPa and 1 GPa, respectively [Krishnan 1998 and Yu 2000]. However, in most of the earlier investigations untreated CNTs or only purified CNTs were used to prepare composite samples and no significant mechanical improvement was observed [Breton 2004]. At present, it is well recognized that in order to maximize the final performance of the material, uniform dispersion of CNTs in polymers and good interfacial adhesion are two critical issues in the fabrication of CNT-polymer composites.

Recently, the PI has demonstrated she is capable of improving the dispersion and compatibility of CNTs



in epoxy systems [Chen and Auad 2006], achieving significant improvement by means of the covalent bonding approach. These first steps are very encouraging for future research in this wide open area.

Figure 1 – SEM micrographs of fractures surfaces (1wt% multi walled CNT): a) unmodified multi walled CNTs-epoxy composite, b) Epoxy modified multi walled CNTs-epoxy composite. [Chen 2006]

Approach:

From a scientific point of view, during the development of the PI's career, two particular systems will be studied in order to provide a unique opportunity to explore the complex field of functionalization of nanotubes.

a) CNTs Addition for Tailorable Vibration Damping Composites: The goal of this project is to design and develop a structural composite with increased damping capacity for use in aeronautical and naval applications. In this work functionalized carbon nanotubes will be used as filler to appropriately tailor acoustic damping responses of structural composite materials. This proposal utilizes new functionalization methods that provide improved bonding with common structural resins (such as epoxies, vinyl esters and unsaturated polyester) thereby enabling stiffer and tougher composites with outstanding acoustic properties. This innovation is applicable to any polymer-based structural material which is subjected to vibration/noise. This research will enable the substitution of metal components, which tend to have inferior acoustic damping properties, with nano-enhanced polymers and composites, with increased stiffness, light weight and superior damping properties.

b) Shape Memory Polyurethane Reinforced with CNTs: The project goals are to improve the behavior and fundamental understanding of shape memory polymers (SMP) based on segmented polyurethanes (PU), reinforced with functionalized carbon nanotubes. During the past years, Dr Auad's research group has examined the synthesis and properties of PU-based SMPs [Marcovich et al 2006, Auad et al 2008]. Figure 2 shows the shape memory recovery of a PU sample warmed at 50°C.

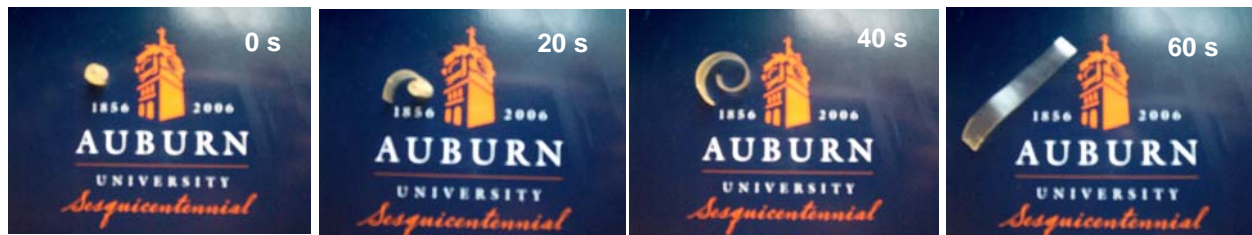


Figure 2 – Shape memory polymer synthesized at Auburn University. Recovery time at 50°C.

The incorporation of nano fillers will lead to the development of a new generation of shape memory material with improved performance characteristics, including improved stiffness, deformation capacity, and recovery force. These nanocomposites are advanced active materials that will be used to create medical devices and biological micro-electro-mechanical systems (MEMS).

From the technological point of view, these two systems will provide a unique opportunity to solve real problems at nano level. This program will explore and identify research issues that can effectively address the limitations of the current technology and provide the engineering society with the knowledge to design high performance materials via nanotechnology.

RESEARCH DESIGN AND METHODOLOGY

The proposed research activities, for both projects, will include: (1) Design, synthesis, and systematic investigation a series of functionalized CNTs in order to achieve novel complex hierarchical nanostructures. (2) Fabrication of well-defined composites using these functionalized CNTs. (3) Development of an understanding of the correlations between the novel nanostructures, the morphology and the physical properties in the final composites.

Several techniques such as microscopy, light scattering, Raman, rheology, and others will effectively elucidate the structural features and physical properties of the nanocomposite materials. The challenge of this proposal is to combine disciplines such as chemistry, materials science, and nano-engineering to provide new technology and fundamental understanding of the mechanisms of nanoparticles interactions

while controlling the molecular behavior through the design of composites. Several graduate and undergraduate students will be involved in the development of this research.

Mid-Project Review Goals:

This project will a) evaluate the feasibility and advantages of engineering nanofibers, CNTs and CNFs-based structural elements for damping and b) broaden and integrate the knowledge of the behavior of SMP-nanocomposites through development of processing-structure-properties relationships.

The project scope includes evaluation of the effects of the selected nanofillers on the matrix properties, optimizing quality control of the starting materials, and the development of process parameters for nanocomposite synthesis.

The specific task for each goal can be summarized as:

a-CNTs Addition for Tailorable Vibration Damping Composites. Our approach to this complex problem consists of two basic stages. i) nanofibers will be identified to achieve the desired nanoreinforcement in the target polymer matrix. During this task we will develop and optimize the nanocomposite preparation to ensure adequate dispersion of the nanofillers; dispersion will be characterized based on rheological and morphological properties. ii) we will evaluate the effects of filler concentration, surface treatments and chemical modification of the selected nanofillers on the mechanical and acoustics properties of glass/epoxy and carbon/epoxy polymer composite. This program will explore and identify research issues that will eventually achieve findings that can effectively address the limitations of the current damping technology and provide the engineering society with the knowledge to design light weight, high performance and high durability dampers via nanotechnology.

b-Shape Memory Polyurethane Reinforced with CNTs: i) synthesis of SMPs with different hard segments and soft segments, ii) preparation of cellulose and chitin whiskers from different sources and characterization of aspect ratio and crystal shape, and iii) preparation and characterization of nanoreinforced SMPs.

Outreach to Industry:

This project will be developed in collaboration with ATS Consulting. This company does ongoing research for the Naval Underwater Warfare Center (NUWC) related to using nanotubes to enhance the acoustic properties for sonar domes. These resources are widely used by transit agencies and their consultants to evaluate and control noise and vibration impacts from transit projects. Examples include de Federal Transit Administration, Federal Railroad Administration, and Urban Mass Transit Administration.

The industry contacts relative to the polyurethane project is: Dr. Vasilis S. Contos, Operations Manager for West Coast Polyurethane Division for BASF Corporation, Orange, California. Additional contacts within the area of medical materials are of enormous importance. Following this direction, results will be disseminated through presentations at professional meetings and peer-reviewed publications. Feedback will be obtained through close cooperation with medical professionals at Auburn School of Pharmacy and College of Veterinary Medicine.

New Resources Required:

We expect to spend part of the money of this proposal in a Four point Resistivity and Conductivity machine that will be used to measure electrical conductivity. The PI also will purchase a Dynamic Light Scattering machine (share base), extensometer for the Universal Testing Machine, FTIR microscope (share base),, chaotic blender (share base),, vacuum oven, and balance.

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BIOGRAPHY SECTION

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Education:

Ph.D. Material Science, University of Mar del Plata, Argentina, (2000)

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Professional Experience:

Assistant Professor, *Auburn University*, Polymer and Fiber Eng. Dep. 2006-present

Research Assistant, *Univ. Southern California*, Dep. Materials Science, 2002-2006

Research Assistant, *California. Institute of Technology*, Chem. Engineering Dep., 2000-2002

Research Interests:

Polymer material science, polymer nanocomposites, flow behavior of polymers, control of microstructures & nanostructure in materials, polymers for structural & biomedical applications.

Representative Publications:

-“Characterization of nanocellulose reinforced shape memory polyurethanes”, M L Auad, VS Contos, S Nutt, M I Aranguren, NE Marcovich, *Polym Int* **57**:651–659 (2008)

-“Improving the Dispersion and Flexural Strength of Multiwalled Carbon Nanotubes-Epoxy Composites through β -Hydroxyester Surface Functionalization Coupled with the Anionic Homopolymerization of the Epoxy Matrix ”, Chen, W., Auad, M.L, Williams, R.J.J., Nutt, S.R., *European Polymer Journal*, volume 42, 10, 2006.

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