Solvay Seminars in Macromolecular Science & Engineering

Macromolecules Innovation Institute (MII)

VIRGINIA TECH

Dr. Todd Alam

"Molecular Level Details of Dynamics, Domain Structure and Transport in Polymers Using NMR Spectroscopy"

Sandia National Laboratories
Principal Research and Development Materials Scientist

Host: Lou Madsen

Abstract: In this seminar, I will provide an overview of the diverse types of research (perhaps NMR centric) that I have recently been involved in at Sandia National Laboratories. As an example, we continue to utilize NMR spectroscopy to probe the dynamics, morphology and transport occurring in polymer materials. The first study involves the development of improved polymer exchange membranes (PEMs) that target specific energy storage applications including fuel cells and batteries. Using ^{1}H double quantum (DQ) NMR spin diffusion (SD) experiments we have measured the nanoscale morphologies for the hydrophilic water/acid domains as a function of water content. The DQ NMR spin diffusion results were tested against proposed structures predicted from molecular dynamics (MD) simulations, as well as used to highlight issues with using simple structural models in analyzing NMR SD results. These spin diffusion results were combined with pulse field gradient (PFG) NMR diffusometry experiments to reveal changes in the water diffusion rate as a function of hydration levels and allow discussion into the impact nanoscale morphology has on the local water transport and proton conductivity in PEMs. The second study involves understanding polymer chain dynamics for a series of epoxy thermosets synthesized utilizing a unique ferrocene-containing amine curing agent pursued to reduce/eliminate cure stress. In crosslinked materials constraints of the polymer chains lead to the formation of residual stresses produced by volumetric shrinkage during cure along with interface stresses resulting from the mismatch in thermal expansion coefficients at adhesion surfaces. We are currently using a variety of different NMR techniques to characterize the molecular level dynamics and processes responsible for the distinct stress reduction and relaxation observed in these ferrocene-containing polymers.

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Bio: **Dr. Todd M. Alam** is a Principal Research and Development Materials Scientist at Sandia National Laboratories and is in an expert in NMR spectroscopy investigations applied to material science. His research interests include the development and utilization of high-resolution solution and solid-state NMR spectroscopy along with pulse field gradient (PFG) NMR diffusometry to characterize a wide range of systems, and to develop a more thorough understanding of the physics and chemistry underlying different observed phenomena or processes. During his tenure at the laboratories, Alam has published extensively in the application of NMR to study polymers, ceramics, glasses, nanomaterials, sol-gels, membranes, inorganic clusters, composites, thin films, and liquid crystals. His recent research interests include the development of high resolution magic angle spinning (HRMAS) NMR diffusometry and multiple-quantum solid state NMR techniques to probe heterogeneous polymer and nanoporous materials.

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