

SMU Department of Mechanical
Engineering
SEMINAR

**“Thermomechanical and Interfacial
Properties of Graphene”**

Professor Rui Huang

*Department of Aerospace Engineering and Engineering
Mechanics, University of Texas at Austin*

Friday, September 20, 2013

3:00 p.m. – 4:00 p.m.

Location: Junkins 110

Abstract: As a two-dimensional crystal membrane, graphene has been found to have many unique physical properties along with a wide range of potential applications. By combining atomistic modeling with continuum theories, we have studied thermomechanical and interfacial properties of graphene. First, the nonlinear elastic properties of graphene at the ground state ($T = 0$ K) are predicted by molecular mechanics simulations, where the in-plane and bending moduli are defined within a general framework of nonlinear continuum mechanics for two-dimensional sheets. The edge effects are discussed for graphene nanoribbons. Next, molecular dynamics simulations are performed to study thermomechanical properties of graphene at finite temperatures ($T > 0$ K). It is found that thermal fluctuation depends nonlinearly on the size of graphene membrane, leading to size dependent thermoelasticity, including negative thermal expansion at low temperatures and temperature-dependent effective elastic modulus at small strain. The results are compared to theoretical analyses based on statistical mechanics of flexible membranes, which further elucidates the effect of temperature in terms of entropic elasticity. Finally, we have developed a simple analytical model for the van der Waals forces between a monolayer graphene and an amorphous substrate, with which a traction-separation relation is derived for the graphene/substrate interface. The effects of surface roughness on adhesion of graphene membranes are discussed along with recent efforts to measure the interfacial properties of graphene experimentally.

Bio: Rui Huang received his Bachelor degree in Theoretical and Applied Mechanics from the University of Science and Technology of China in 1994 and his PhD degree in Civil and Environmental Engineering, with specialty in Mechanics, Materials, and Structures, from Princeton University in 2001. He joined the University of Texas at Austin as an Assistant Professor in September 2002 and was promoted to Associate Professor with tenure in 2008.

He currently holds the endowed position of Pearlie Dashiell Henderson Centennial Fellowship in Engineering at UT Austin.