

Wednesday Morning, November 2, 2011

Graphene and Related Materials Focus Topic

Room: 208 - Session GR+MN-WeM

Graphene: Mechanical and Thermal Properties, Graphene MEMS and NEMS

Moderator: J. Rabe, Humboldt University Berlin, Germany

8:00am **GR+MN-WeM1 Graphene Atomic Membranes: From Patchwork Quilts to Atomic Drums, P.L. McEuen**, Cornell University
INVITED

Graphene is the world's first atomic membrane, a robust, one-atom thick freestanding layer of sp²-bonded carbon. The physical properties of these membranes straddle the border between soft and hard condensed matter. They are strong but highly flexible, with bending stiffness comparable to a lipid bilayer but stretching stiffness similar to diamond. Meter-scale polycrystalline graphene films can now be produced cheaply and easily, opening the door to applications in both science and technology. In this talk we will present new results on the structural and physical properties of this remarkable 2D material, including the first STEM images of graphene grain boundaries and the patchwork-quilt-like structure of graphene grains. We also discuss experiments on atomic drums made with graphene membranes that can be actuated and probed either electrically or optically. Unlike for traditional MEMS and NEMS, we find that stiction and entropy are key parameters in determining the drum's vibration frequency.

8:40am **GR+MN-WeM3 Nanomechanics of Graphene: Non-Linear Response, Fracture, and Crack Propagation, R. Perriot, Y. Lin**, University of South Florida, X. Gu, Aalto University School of Science and Technology, Finland, V.V. Zhakhovsky, I.I. Oleynik, University of South Florida

Recent nanoindentation experiments on graphene have revealed its exceptional strength, making it an excellent candidate for the design of nano devices such as MEMS and pressure sensors. Therefore, it is critical to understand the mechanical properties of graphene, and its response to a wide range of loading pressures beyond the elastic regime. In this work we performed molecular dynamics (MD) simulations of the nanoindentation of graphene membranes by a spherical indenter. The indentation curves (load vs. indentation depth) obtained from simulations revealed two regimes of response: linear for smaller, and non-linear for larger indentation depths respectively. The MD results are in good agreement with the theory of elastic plates and recent experiments. Using the kinetic theory of fracture, we were able to determine the breaking strength of graphene and its dependence on the indenter radius. MD simulations also provided an atomic-scale description of the breaking process, which occurs through crack formation and propagation in graphene.

9:00am **GR+MN-WeM4 The Effect of the Environment on Electrical and Mechanical Properties of Graphene, K. Bolotin**, Vanderbilt University

Every atom of graphene, a monolayer of graphite, belongs to the surface. Therefore, the environment of graphene -- the substrate onto which graphene is deposited and the coating on top of graphene -- intimately affects the properties of graphene. In this talk, we demonstrate that both mechanical and electrical properties of graphene can be tuned by varying the environment of graphene.

To study the mechanical properties of graphene, we developed a novel technique that is based on measuring the temperature-dependent deflection of a "bimetallic" cantilever composed of graphene and silicon nitride or gold layers. We demonstrate that the built-in strain, the substrate adhesion force and even the thermal expansion coefficient of graphene depend on the substrate under it.

To study the electrical properties of graphene in various environments, we developed a technique to fabricate electrically contacted multiterminal *suspended* graphene devices that are submerged into liquids. We explore the dependence of electron mobility of graphene on dielectric constant and ionic concentration of liquids surrounding graphene. We find that ions in liquids can cause strong scattering in graphene and that very large values of mobility (>40,000 cm²/Vs) can be achieved in ion-free liquids.

9:20am **GR+MN-WeM5 Nanoscale Friction and Adhesion Behavior of Graphene: The Effect of Sliding History, X.-Z. Liu, Q. Li, B. Zhang, R.W. Carpick**, University of Pennsylvania

As a prominent example of a two-dimensional (2-D) material, graphene has drawn much attention because of its extraordinary physical properties.

However, in contrast to its electronic and thermal properties, the mechanical and tribological properties of graphene remained poorly understood. These properties are interesting scientifically because of the extremely high strength and low defect density of the bonds, and the intrinsically wrinkled structure of graphene. These properties are important for integrating graphene with devices. We studied the friction and adhesion between nanoscale single-asperity tips and exfoliated graphene sheets using atomic force microscopy (AFM). We have previously reported that friction on few-layer graphene (and other 2-D materials) depends on the number of layers[1], whereby the friction is higher for fewer layers. The layer-dependence is associated with the presence of a "strengthening" effect, where the static friction force builds up as scanning proceeds, most evident for the thinnest layers. This suggested that the increase was due to the build-up of a puckered area in front of the tip due to the high compliance of the graphene and adhesion with the tip. However, adhesion between the tip and graphene, measured by regular AFM force-displacement spectroscopy, does not change appreciably when the layer number changes. This result agrees with trends obtained from finite element method (FEM) simulations. However, we observed that both friction and adhesion exhibit a contact history dependence. For friction on single layer graphene, the strengthening is not present initially, but rather, it gradually builds up as the tip is rastered over the surface. This suggests that the puckered structure requires repeated scanning before it geometrically develops to a point where friction is enhanced. In addition, we find that adhesion is enhanced if it is measured without breaking the tip-graphene contact after sliding the AFM tip over the same area for a sufficient distance. This sliding-history dependence was not observed on bulk graphite or SiO₂ substrates, and thus appears to be yet another unique feature of the tribological behavior of atomic sheets. These two observations strongly suggest that the geometric structure of the sheet and the contact area it makes with the tip is significantly affected by the sliding history.

[1] Lee, C., Q. Li, W. Kalb, X. Liu, H. Berger, R. Carpick, and J. Hone, *Frictional Characteristics of Atomically Thin Sheets*. Science, 2010. **328** (5974): p. 76.

10:40am **GR+MN-WeM9 Molecular Dynamics Simulations of Melting of Graphene, B. Steele, V.V. Zhakhovsky, R. Perriot, I.I. Oleynik**, University of South Florida

It has long been predicted by Peierls, Landau, and Mermin that infinite two-dimensional solids are unstable and should melt at any finite temperature. The stability of graphene, a two-dimensional layer of carbon atoms, is thus explained by the presence of an additional degree of freedom that allows it to buckle in the third direction normal to the 2-D perfect plane. We performed large-scale molecular dynamics (MD) simulations of graphene melting in order to provide a fundamental insight into the stability of graphene, as well as to investigate the nature of the defects naturally created by thermal excitations at high temperatures. We will discuss the types of defects appearing before melting, the atomic-scale mechanisms of melting, and the nature of the resulting carbon melt. In addition, the graphene melting in 3D space *versus* 2D-constrained melting is also discussed. The importance of a proper description of chemical bonding in graphene at high temperatures is illustrated using different interatomic potentials: the reactive bond order (REBO) potential and the newly developed screened environment dependent SED-REBO. Comparisons with other recent simulations of graphene melting (including those using the LCBOPII potential for carbon) are also presented.

11:00am **GR+MN-WeM10 Inhomogeneous Strain in Monolayer Epitaxial Graphene, D.A. Schmidt**, Ruhr-University Bochum, Germany, T. Ohta, L.B. Biedermann, T.E. Beechem, S.W. Howell, G.L. Kellogg, Sandia National Laboratories

We report a large in-plane compressive strain (up to 0.5%) and its inhomogeneous variation at micrometer length scale in single layer graphene films on silicon-carbide (SiC) (0001). The strain, due to the difference in lattice constants and thermal expansion coefficients of graphene and SiC substrate, is probed using Raman scattering. We show that both the growth mechanism and the relaxation along the mismatched symmetry of the graphene and underlying substrate can affect the exact amount of local strain. The large compressive strain implies that monolayer graphene is tightly grafted to the underlying interface layer and SiC substrate; otherwise it would delaminate to relieve the strain. The magnitudes of the structural strain and its local variation are significant and

need to be taken into account for electronics applications based on the graphene-SiC(0001) system.

The Raman microscope was supported under BMBF grants 05KS7PC2. D. A. S acknowledges support within the BMBF funded projects 05KS7PC2 and 05K10PCA. The work was also supported in part by the LDRD program at SNL and the US DOE Office of Basic Energy Sciences' Division of Materials Science and Engineering (Contract No. DE-AC04-94AL85000). Part of this work was performed at CINT (Contract No. DE-AC04-94AL85000). SNL is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Authors Index

Bold page numbers indicate the presenter

— B —

Beechem, T.E.: GR+MN-WeM10, 1
Biedermann, L.B.: GR+MN-WeM10, 1
Bolotin, K.: GR+MN-WeM4, **1**

— C —

Carpick, R.W.: GR+MN-WeM5, 1

— G —

Gu, X.: GR+MN-WeM3, 1

— H —

Howell, S.W.: GR+MN-WeM10, 1

— K —

Kellogg, G.L.: GR+MN-WeM10, 1

— L —

Li, Q.: GR+MN-WeM5, 1
Lin, Y.: GR+MN-WeM3, 1
Liu, X.-Z.: GR+MN-WeM5, **1**

— M —

McEuen, P.L.: GR+MN-WeM1, **1**

— O —

Ohta, T.: GR+MN-WeM10, 1

Oleynik, I.I.: GR+MN-WeM3, 1; GR+MN-WeM9,
1

— P —

Perriot, R.: GR+MN-WeM3, **1**; GR+MN-WeM9, 1

— S —

Schmidt, D.A.: GR+MN-WeM10, **1**
Steele, B.: GR+MN-WeM9, **1**

— Z —

Zhakhovsky, V.V.: GR+MN-WeM3, 1; GR+MN-
WeM9, 1
Zhang, B.: GR+MN-WeM5, 1