Advanced Course to be held at the
International Centre for Mechanical Sciences (CISM)

Structure and Multiscale Mechanics of Carbon Nanomaterials

July 21-25.2014

Coordinator:
Prof. Dr. Oskar Paris
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LECTURERS (in alphabetic order)

Prof. Dr. Claudia Draxl
Institute of Physics, Humboldt Universät Berlin, Germany
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6 lectures: Ab-initio methodology, density-functional theory including van der Waals interaction, many-body perturbation theory to describe electronic structure and excitations (photoemission, optical absorption, Raman scattering, XANES, etc.). One lecture will be dedicated to elastic and mechanical properties. The remaining time will go to applications.

Prof. Dr. David Dunstan
School of Physics and Astronomy, Queen Mary University of London
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6 lectures: Overview of high pressure methods and Raman spectroscopy; Overview of nanomechanical testing methods. Pressure response of nanotubes with attention to the variables (single and multiple walls, bundling, pressure medium, excitation, etc); Collapse of nanotubes at very high pressures; Comparison of experimental data and theory, with an emphasis on the unsolved questions.

Dr. Siddhartha Pathak
Center for Integrated Nanotechnologies
Los Alamos National Laboratory
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6 lectures: Overview of nanomechanical testing methods (2 lectures). Mechanical Behavior of Carbon Nanotubes: from a Single Tube towards Complex Networks (4 lectures). One lecture will cover the diversity of CNTs, mechanical deformation of single CNTs and non-interacting multiple CNTs. Remaining three will focus on the mechanical deformation of vertically aligned CNTs (VACNTs). The lectures on VACNTs will compare the various
synthesis techniques of VACNTs (such as carbide derived carbon, and chemical vapor deposition) and their resultant large variation in structure and properties (porosity, CNT tube thickness, modulus, buckling strength), their large scale deformation and buckling behavior, viscoelasticity and potential applications.

Dr. Markus Hartmann
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6 lectures: Introduction into atomistic Monte Carlo and Molecular Dynamics simulation techniques and their application to the mechanical modeling of carbon nanostructures. Special emphasis will be put on bridging the scale from atomistic simulations to continuum modeling. Structures that will be discussed are graphene, nanotubes and fullerenes.

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6 lectures: Basic overview on carbon nanostructures; Synthesis, structure and applications of carbon nanomaterials (nanotubes, nanodiamond, graphene, and porous carbons). Structure of carbon fibers and other disordered carbon nanomaterials; Overview on experimental methods to characterize carbon nanostructures; X-ray diffraction applied to carbon nanostructures; in-situ mechanical experiments, micro-and nanobeam diffraction.

Prof. Dr. Bob Young
School of Materials, University of Manchester
Oxford Road, Manchester, M13 9PL, UK
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6 lectures: Stress-induced Raman band shifts in carbon materials; Deformation of carbon fibres and composite micromechanics; Deformation of carbon nanotubes; Carbon nanotube nanocomposites; Deformation of graphene; Graphene nanocomposites.

Time Table

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Outline and Objectives

Carbon is often designated as *The Material* of the 21st century. Graphene, carbon nanotubes, fullerenes and other highly organized carbon nanostructures are under investigation worldwide for advanced functional materials in diverse fields. Carbon nanomaterials play a key role in modern energy storage devices such as Lithium-ion batteries, super capacitors, or fuel cells; they are thought to have the potential to revolutionize electronics by at least partly replacing silicon technology by carbon technology; and most importantly in the present context, they have extraordinary mechanical properties. The strong covalent bonding between sp² hybridized carbon atoms leads to materials with unsurpassed stiffness and strength. Graphene is known to be the strongest material ever tested with a tensile strength 200 times greater than that of steel and a tensile modulus beyond 1000 GPa. Although the graphene hammock carrying a whole cat is still a rather theoretical concept, there are already many potential mechanical applications envisaged with this unique material. Similar prospects hold also true for its rolled-up versions in 1D (nanotubes) and 2D (fullerenes). Beside these “modern” highly ordered carbon nanomaterials, there exist a broad variety of more disordered carbons with properties which are also largely determined by their nanostructure. From crystalline graphite to fully amorphous (glassy) carbon, a whole continuum of partly disordered, defect rich materials such as carbon (nano) fibers, carbon black, activated carbons, etc. are widely used in diverse applications and they are continuously improved. Modern carbon fibers for instance almost reach the tensile modulus of graphene, and their tensile strength can be more than 6 GPa, which is yet an order of magnitude larger than that of a typical steel. These outstanding mechanical properties of carbon materials are not only useful for structural applications (e.g. in composites), they are also of critical importance for the mechanical integrity of essentially all functional devices based on them.

This CISM course aims at providing a broad overview on the relationship between structure and mechanical properties of carbon nanomaterials from world-leading scientists in the field. The main goal is to get an in-depth understanding of the exceptional broad range of mechanical properties of carbon materials based on their unique nanostructure and on defects of several types and at different length scales. For instance, in basically sp² bonded carbons the role of curvature as well as in plane defects (e.g. 5-ring structures in fullerenes, 5-7-ring structures known as Stone-Wale defects, etc.), and out-of-plane “covalent” cross-links between graphene planes are known to strongly influence their mechanical behavior. In larger structures such as carbon fibers, not only such atomic defects, but also the preferred orientation and the cross-sectional texture of multilayer-graphene crystallites, as well as their size and anisotropy are responsible for a wide range in stiffness and strength under tensile and compressive loads. The main goal of the present CISM course is to provide a comprehensive and modern view on how targeted design of carbon based materials with specific mechanical properties can be reached by controlling nanostructure and defects at several scales of hierarchy.

The course will cover a broad range of nanomaterials such as graphene, single-wall- and multi-wall carbon nanotubes, fullerenes, carbon onions, nanodiamonds, carbon fibers, mesoporous carbons etc.. One particular focus will be on the multiscale modeling of mechanical properties of such materials using *ab-initio* DFT calculations (including van der Waals interactions), atomistic simulations with Molecular Dynamics (MD) and Monte Carlo (MC) methods, as well as continuum mechanical approaches. Experimental lectures will cover many aspects of carbon nanostructures, such as their synthesis, their structure at several length scales, their mechanical properties, and their application potential in diverse fields. Special emphasis will be put on sophisticated experimental methods to assess the relationships between structure and mechanical properties at different scales. Micro- and nanomechanical testing, advanced Raman scattering, and X-ray scattering using microbeam synchrotron radiation are among the techniques that will be covered in the course. Moreover, in-situ mechanical testing in combination with the above and other techniques will be considered. Besides the many carbon nanomaterials themselves, the course will also include composites with these materials as reinforcing fibers or nanoparticles.

The course should be of particular interest for PhD students and Postdocs working in a
specific field of carbon nanomaterials and/or –nanocomposites to widen their horizon beyond their specific topic. Materials scientists, physicists and chemists are the attendees particularly expected, but the course might also be of interest for mechanical and electrical engineers, and for researchers working in the fields of nanotechnology and biomedical engineering. Although the basic concepts will be covered by introductory lectures, it is expected that the attendees have at least some basic knowledge on mechanical concepts and on the physics of nanomaterials.

**Suggested preliminary reading**

P. Morgan: Carbon Fibres and their composites, CRC Press Inc, 2005


