Workshop on Computational Materials Design

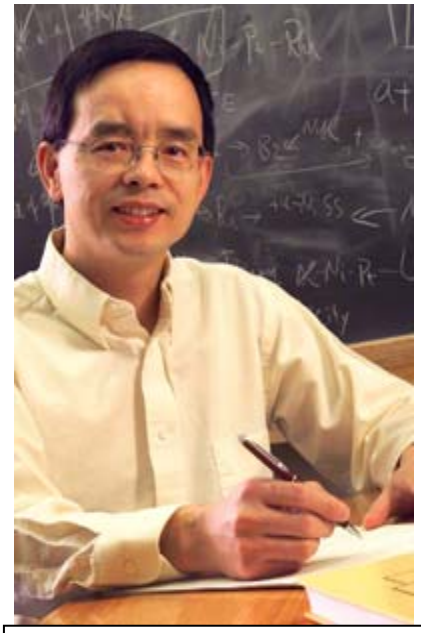
December 09, 2009
Penn State University
The Nittany Lion Inn

Faculty and Guest Speaker Research Abstract

Table of Contents

Zi-Kui Liu 2
David L. McDowell 3
Edward Vincent Clancy, JD., D.Eng. MBA, Esq. 4
Long-Qing Chen 5
Qiang Du 6
Padma Raghavan 7

Zi-Kui Liu
Penn State University
Professor of Materials Science and Engineering
Director, Center for Computational Materials Design



Research Interests:

- First-principles calculations
- Computational thermodynamics
- System materials design
- Aluminum alloys
- Hydrogen storage materials
- Magnesium alloys
- Nickel alloys
- Perovskites
- Steels

Research interests are on the design and simulation of a wide range of materials through integrating first-principles calculations, thermodynamic/kinetic modeling, and critically designed experiments for structural and functional applications.

Recent studies in Professor Liu's Phase Research Lab focus on aluminum alloys, magnesium alloys, Ni-base superalloys, and peroveskites. The primary emphasize is on fundamentals of phase stability and their applications in understanding and designing materials chemistry, processing and properties.

Research activities are supported by both federal funding agencies such as National Science Foundation, Office of Naval Research, and Department of Energy, and industrial companies such as USCAR, Kennametal, Inc., ExxonMobil Research & Engineering Co., Air Products and Chemicals, Inc.

Prof. Liu has created and serves as Director of National Science Foundation Industry/University Cooperative Research Center for Computational Materials Design with the support of national laboratories and manufacture companies in the United States, jointly with Georgia Institute of Technology. The center aims to educate the next generation of scientists and engineers with a broad, industrially relevant perspective on engineering research and practice.

David L. McDowell
Georgia Institute of Technology
Regents' Professor and Carter N. Paden, Jr. Distinguished Chair in Metals Processing
Co-Director, Center for Computational Materials Design

Research Interests:

- Mechanics of Materials and Computer-Aided Engineering and Design
- Material deformation and damage, constitutive laws, and metals processing

Dr. David L. McDowell received his M.S. and Ph.D. in Mechanical Engineering from the University of Illinois in 1981 and 1983, respectively. Dr. McDowell is Regents' Professor and Carter N. Paden, Jr. Distinguished Chair in Metals Processing in the School of Materials Science and Engineering and the Woodruff School of Mechanical Engineering at Georgia Tech. At Tech, he has served as Director of the Mechanical Properties Research Laboratory since 1992, and as Chair of the Materials Council since 1994. McDowell's research focuses on the synthesis of experiment and computation to develop physically-based constitutive models for nonlinear and time-dependent behavior of materials, with emphasis on wrought and cast alloy systems. Phenomena of interest include cyclic plasticity and fatigue, finite strain plasticity, defect field theories, behavior of foams and honeycomb materials, microstructurally small fatigue crack behavior, creep-fatigue -environment interaction, time-dependent fracture, nano-mechanics with focus on interfaces, and multiscale modeling.

As Co-Director of the NSF-sponsored Center for Computational Materials Design, a joint Penn State-Georgia Tech I/UCRC, he is actively pursuing development of strategies for multifunctional design of materials. McDowell currently serves on the editorial boards of several journals, and is co-Editor of the International Journal of Fatigue. A Fellow of SES, ASM International, and ASME, David is a recipient of the 1997 ASME Materials Division Nadai Award for career achievement and the 2008 Khan International Medal for lifelong contributions to the field of metal plasticity.

Edward Vincent Clancy, JD., D.Eng. MBA, Esq.

Guest Speaker

Dr. Ed Clancy is Chief Technology Officer of ACTA LLC (Advanced Cooling Technology Applications – www.acta-llc.com), a nanotech startup firm located in Boulder, Colorado. ACTA has a patented process on nanofluids that improves heat transfer properties of refrigerants and is working with Penn State and the University of Cincinnati in developing this technology. ACTA is also working with Ball Aerospace & Technology on a SBIR contract with the Air Force on improving heat pipes that cool electronics using nanofluids. Recently eSpace, an accelerator for high tech businesses located in Colorado, started working with ACTA. Prior to starting ACTA in February 2009, Ed worked as a patent attorney for the USPTO. Dr. Clancy served as Program Director at the National Science Foundation for the Industry / University Cooperative Research Centers in the Industrial Innovation Partnership Division (2005-2007). Ed Clancy is professor emeritus of engineering from Cal Poly (Pomona). He has been a faculty researcher at Department of Energy (DOE) UC Berkeley lab and the US Navy's David Taylor Lab. Professor Clancy retired from the US Navy as a CAPTAIN. He is a licensed professional engineer and attorney in California and Colorado. Ed is also a licensed Patent Attorney for the USPTO.

Long-Qing Chen

Penn State University
Professor of Materials Science and Engineering
Faculty, Center for Computational Materials Design

Research Interests:

- Thermodynamics and kinetics of phase transformations
- Phase-field simulation of domain structure and microstructure evolution
- Ferroelectric thin films
- Alloy precipitations
- Martensitic transformations
- Interactions between defect and phase microstructures
- Multiscale modeling

Dr. Chen's main research interest is in the fundamental understanding of the thermodynamics and kinetics of phase transformations and mesoscale microstructure evolution in bulk solid and thin films using computer simulations. Essentially all engineering materials contain certain types of microstructures, and our success of designing new materials is largely dependent on our ability to control them. Microstructure is a general term that refers to a spatial distribution of structural features that can be phases of different compositions and/or crystal structures, or grains of different orientations, or domains of different structural variants, or domains of different electrical or magnetic polarizations, as well as structural defects such as dislocations. It is the size, shape, and spatial arrangement of the local structural features that determine the physical properties of a material such as mechanical, electrical, magnetic and optical properties. For the last decade, Dr. Chen's group at Penn State is particularly active in developing phase-field models for microstructure evolution during various materials processes including grain growth, coherent precipitation, ferroelectric domain formation, particle coarsening, domain structure evolution in thin films, phase transformation in the presence of structural defects, and effect of stress on microstructure evolution. Current research focus is on the effect of stress/strain on ferroelectric phase transitions and domain structure evolution in ferroelectric and multiferroic thin films, domain structures in ferromagnetic shape memory alloys, precipitate microstructure evolution in Al- and Ni-alloys, strain-dominated morphological evolution, effect of defects such as dislocations on microstructure evolution. Dr. Chen's group collaborates extensively with experimentalists and with industry.

Qiang Du
Penn State University
Professor of Mathematics and Materials Sciences
Faculty, Center for Computational Materials Design

Research Interests:

• Numerical Algorithms

• Partial Differential Equations

• Parallel Computation

• Scientific computation applications in physical, biological and materials sciences

• data and image analysis

Dr. Du's research is mostly focused on developing efficient and robust mathematical models and simulation codes for various problems in computational materials science, including efficient meshing, high order discretization methods and fast solutions.

Professional experience:

- 2006 Verne M. Willaman Professor of Mathematics, Penn State University
- 2001 Professor of Mathematics, Penn State University
- 1996-2001 Senior Lecturer and Professor, HKUST
- 1999 Professor, Iowa State University
- 1992 Visiting Associate Professor, Carnegie Mellon University
- 1990-1996 Assistant and Associate Professor, Michigan State Univ.
- 1990 Faculty research participation, Argonne National Lab
- 1988-1990 Dickson Instructor, University of Chicago
- 1988 Research Assistant, Los Alamos National Lab
- 1983 S.S.Chern Program, Academia Sinica (selected by AMS-SIAM committee)

Padma Raghavan
Penn State University
Director, Institute for CyberScience
Professor, Computer Science and Engineering
Faculty, Center for Computational Materials Design

Padma Raghavan is a Professor of Computer Science and Engineering at the Pennsylvania State University. In 2007, Raghavan was appointed the first Director of the Institute for CyberScience at Penn State to promote multidisciplinary research and education in discovery and design through computation, mathematical modeling and data analysis. Raghavan's research concerns high-performance computing and computational science and has over 75 publications in these areas including "Parallel Processing for Scientific Computing", an edited volume published by SIAM in 2006. In recognition of her contributions to high performance computing, Raghavan received the CAREER award from NSF and the Maria-Geoppert Mayer Distinguished Scholar Award from the University of Chicago and the Argonne National Laboratory. Raghavan currently serves on the editorial board of the SIAM Journal on Scientific Computing and on the program committees of many major conferences sponsored by ACM, IEEE or SIAM. Raghavan will co-chair the 2011 SIAM Conference on Computational Science and Engineering.