Yale Institute for Nanoscience and Quantum Engineering

Friday- September 13, 2013

12:00 to 1:00 p.m.

Becton Seminar Room

Light lunch will be served at 11:45 a.m.

Professor Corey O'Hern

Departments of Mechanical Engineering & Materials Science, Applied Physics, and Physics
Yale University

"What determines the glass-forming ability of metallic alloys?"

I will describe our recent computational studies of model bulk metallic glasses to understand the features that differentiate good from poor glass-forming alloys. Good glass-formers possess low critical cooling rates, below which the system crystallizes. In contrast, poor glass-formers possess high critical cooling rates and small critical sample thicknesses. We determine the atomic size ratios, stoichiometries, binding energies, and heats of mixing that maximize the glass-forming ability of model binary Lennard-Jones systems. In addition, using genetic algorithms, we identify the optimal crystal structures for each atomic size ratio and stoichiometry to determine how the packing efficiency difference between the crystal and glass affect the glass-forming ability of each alloy. These studies represent a key first step toward computational design of novel bulk metallic glasses.

Professor Udo D. Schwarz

Department of Chemical Engineering& Mechanical Engineering, Yale University

" Evolving Atomic-resolution Scanning Probe Microscopy: Towards Quantitative, Chemically Selective 3D Imaging "

Despite the evolution of scanning probe microscopy (SPM) into a powerful set of techniques that image surfaces and map their properties down to the atomic level, significant limitations in both imaging and mapping persist. Currently, typical SPM capabilities qualitatively record only one property at a time and at a fixed distance from the surface. Furthermore, the probing tip's apex is chemically and electronically undefined, complicating data interpretation. To overcome these limitations, we started to integrate significant extensions to existing SPM approaches. First, we extended noncontact atomic force microscopy with atomic resolution to three dimensions by adding the capability to quantify the tip-sample force fields near a surface with picometer and piconewton resolution. Next, we gained electronic information by recording the tunneling current simultaneously with the force interaction. We then moved on to study the influence of tip chemistry and asymmetry on the recorded interactions. Applications to metal oxides are presented. From this platform, we present our vision of a method capable of characterizing full atomic-scale chemical and electronic properties.

HOST: Paul Fleury