short course

TMS2012
141st Annual Meeting & Exhibition

March 11 – 15, 2012 • Walt Disney World Swan & Dolphin Resort • Orlando, Florida

Existing and Needed Computational Capabilities of Ni-base Superalloys

Organized by Center for Computational Materials Design (www.ccmd.psu.edu)

Sunday, March 11, 2012 • 8:30 a.m. – 5:00 p.m.

Member fee: **$250**
Late Member fee: **$300**
Nonmember fee: **$325**
Late Nonmember fee: **$375**

Course Description and Objectives:
Assess the existing and needed modeling capabilities for Ni-base superalloys in U.S. universities, research institutions, and industry applicable to the Materials Genome Initiative. In this context "the word genome, when applied in non-biological contexts, connotes a fundamental building block toward a larger purpose." The workshop will chart the future development of fundamental computational tools that can be tailored to specific applications with minimum modification.

Tentative topics:
Fundamentally, the building blocks of materials are individual phases and their interfaces as a function of temperature, pressure, and composition. These are thus intrinsic to the Materials Genome concept and examples of the development of models using these constructs for Ni Superalloys will be provided in the workshop:

1. Overview of modeling strategies, scales of material hierarchy, verification and validation
2. Commercial alloys based on individual phase information
   - 2.1. Relevant models and scales for strength
   - 2.2. Relevant models and scales for fatigue
   - 2.3. Relevant models and scales for creep and oxidation
3. Role of microstructure and interfaces
   - 3.1. Microstructure simulations
   - 3.2. Microstructure representation and inverse correlations
   - 3.3. Interfaces and models - APBs, stacking faults, GBs, twins, and slip transfer.
4. First principles and modeling of computable properties

Who should attend:
Scientists and engineers working on or interested in computational modeling of alloys.

Instructors:
Zi-Kui Liu, David McDowell, Rollie Dutton, Samuel Thamboo, Long-Qing Chen, Rick Neu, and ***Greg Olson***