PURDUE UNIVERSITY

PURDUE MATERIALS ENGINEERING

Materials Engineering Fall 2014 Seminar Series

Friday, Oct. 24th
3:30 pm Coffee
3:45 pm Seminar
ARMS 1010

Materials Genome® and Entropy

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The word genome, when applied in non-biological contexts, connotes a fundamental building block toward a larger purpose [1]. The materials genome is encoded in the language of CALPHAD databases [2], in which the properties of individual phases are modeled and used for processing and materials design [3-4]. In this presentation, the recent and future developments in the field are discussed [5-6]. Furthermore, our newly developed approach in predicting property anomalies is reviewed in term of first-principles calculations and classic and statistic thermodynamics, particularly entropy, with thermal expansion as an example [7-8].

1. National Science and Technology Council, "Materials Genome Initiative for Global Competitiveness," *http://www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf Office of Science and Technology Policy, Washington DC*, June, 2011.
2. L. Kaufman and J. Agren, "CALPHAD, first and second generation - Birth of the materials genome," *Scr. Mater.,* Vol.70, 2014, 3-6.
3. Z. K. Liu, D. G. Schlom, Q. Li and X. X. Xi, "Thermodynamics of the Mg-B system: Implications for the deposition of MgB2 thin films," *Applied Physics Letters,* Vol.78, 2001, 3678-3680.
4. G. B. Olson and C. J. Kuehmann, "Materials genomics: From CALPHAD to flight," *Scr. Mater.,* Vol.70, 2014, 25-30.
5. Z. K. Liu, "First-Principles Calculations and CALPHAD Modeling of Thermodynamics," *Journal of Phase Equilibria and Diffusion,* Vol.30, 2009, 517-534.
6. C. E. Campbell, U. R. Kattner and Z. K. Liu, "File and data repositories for Next Generation CALPHAD," *Scr. Mater.,* Vol.70, 2014, 7-11.
7. Z. K. Liu, Y. Wang and S. L. Shang, "Origin of negative thermal expansion phenomenon in solids," *Scr. Mater.,* Vol.65, 2011, 664-667.
8. Z. K. Liu, Y. Wang and S. L. Shang, "Thermal Expansion Anomaly Regulated by Entropy," *Sci Rep,* 2014, in review.

Dr. Zi-Kui Liu is a Professor of Materials Science and Engineering at The Pennsylvania State University (http://www.matse.psu.edu/faculty/liu). He obtained his BS from Central South University (China), MS from University of Science and Technology Beijing (China), PhD from Royal Institute of Technology (Sweden). He was a research associate at University of Wisconsin-Madison and a senior research scientist at Questek Innovation, LLC. He has been at the Pennsylvania State University since 1999 and the Editor-in-Chief of CALPHAD journal since 2001. Dr. Liu is a Fellow and Board of Trustee of ASM International and was a member of the TMS Board of Directors. He received the TMS Brimacombe Medalist Award, ACers Spriggs Phase Equilibria Award, and the ASM J. Willard Gibbs Phase Equilibria Award.

Dr. Liu's current research activities are centered on first-principles calculations, modeling of thermodynamic and kinetic properties, and their integration in understanding defects, phase stability, and phase transformations, and designing and tailoring materials processing and properties. He is the founder and the director of Center for Computational Materials Design (www.ccmd.psu.edu) and has published over 340 papers in peer-reviewed journals (http://scholar.google.com/citations?user=XEkppu4AAAAJ&hl=en, http://www.researcherid.com/rid/A-8196-2009). His group web site is at www.phases.psu.edu.