CHiMaD | Center for Hierarchical Materials Design

SPECIAL SEMINAR

A COMPUTATIONAL APPROACH TO MATERIALS DESIGN

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June 2, 2014 (Monday)
COOK Hall, Rm 2058 | **4.00pm-5.00pm**
Cookies & Coffee will be provided.

ABSTRACT In order to reduce the number of the alloy design cycles, a theoretical approach, which includes CALPHAD models and plastic deformation models, is proposed to bridge the gaps among processing-structure-properties. The enumerative calculations are then leaded by Genetic Algorithms (GAs) for more effective search in multi-dimensional chemical composition and heat treatment space to improve the material properties. A design of low alloy addition TRIP-assisted steel is demonstrated as an example: to improve the work to necking at room temperature. The inputs, including the chemical composition and the heat-treated temperatures, are optimized to improve the mechanical properties. The sequence of the material selection is recommended as (1)C (2)Si and (3)Mn and the heat treated temperatures can be decided accordingly.

Shengyen Li is the PREP Post-Doc researcher at National Institute of Standards and Technology – NIST, in Gaithersburg, MD. The focus of his work is on the material informatics and potential applications for material design, superalloys especially. Before joining NIST, Shengyen proposed the computational approach for high performance TRIP steel and received his PhD degree from Texas A&M University from 2008 to 2013. In scientific area, Shengyen is interested in microstructure evolution either during the processing or under the mechanical field. He is also enthusiastic about the application of the theoretical models with computational techniques, such as CALPHAD, Computational Algorithms, and machine techniques etc.