CHiMaD | Center for Hierarchical Materials Design

SPECIAL SEMINAR

INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING AND THE MATERIALS GENOME INITIATIVE:

ACTIVIES AT THE HERO-m CENTER

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December 4, 2014 (Thursday)
COOK Hall, Rm 2058 | **12.00pm-1.00pm**

ABSTRACT The concept of integrated computational materials engineering (ICME) has emerged over the last decade as a powerful method to design materials for targeted performance and it has been defined as "… the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation". With materials information is meant curated data sets, structure-property models, processing-structure relationships, physical properties and thermodynamic, kinetic and structural information. Within ICME there is a need for databases to be used in models and computational tools, the materials genome, which may be defined as a set of information (models and databases) allowing prediction of materials structure and properties as well as their response to processing and usage conditions.

The Hero-m center was launched in 2007 as a collaborative effort between KTH and Swedish industry with the aim of developing the methods for materials design along the principles of ICME. The mission is to develop the tools and competence for fast, intelligent and cost efficient materials development for Swedish industry. The center is funded jointly by Swedish VINNOVA, the industrial partners and KTH and the total budget is ca 200 MSEK over a period of 10 years.

The talk will present some of the activities within Hero-m in the area of ICME and the materials genome.

Annika Borgenstam *is professor in Micro and Nano structures in Alloys at the Department of Materials Science and Engineering at KTH Royal Institute of Technology in Stockholm, Sweden. Her work is on the structure of metallic materials from nano- to micro level, focusing on the understanding of how a particular structure is formed and how it can be modified. The emphasis is on the theoretical and experimental analysis of these structural transformations, with particular focus on the link between thermodynamic and kinetic properties and transformation mechanisms. The main objective is to develop models that describe how the structures are formed which can be used in the design of new materials or to improve already existing materials. Although the models are the focus, it is necessary to work experimentally to increase the understanding of the transformations that are to be described, as well as to verify developed models.*