INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

Friday, 31 May, 1:00 p.m.
Room IC 02-718

Dr. Ursula R. Kattner

Materials Science and Engineering Division
National Institute of Standards and Technology
Gaithersburg, USA

CALPHAD modeling, moving forward

The CALPHAD method is an essential part of computational materials and process development, and many commercial CALPHAD databases are available for this purpose. The history of the CALPHAD method is also the history of constant model improvement and increasing sophistication. Recent efforts are in improving the description of the unaries and increasing incorporation of results from density functional theory which provide the data needed for intricate and accurate modeling of the phases.

These data, along with improved model formalisms for the composition dependence, make simplifications less necessary allowing reliable descriptions of multicomponent systems that are increasingly based on extrapolations of binary descriptions while reducing the number or required parameter values. Simultaneously the CALPHAD method is being expanded for the modeling of all kinds of other phase-based properties. For example, the molar volume is a property that is needed for the simulation of numerous materials processes but it has been included only in a handful of proprietary CALPHAD databases. Several assessments of the temperature dependence of the molar volume of the pure elements have been published in the literature using different formalisms. Some of these formalisms are only meaningful when used with the currently accepted lattice stabilities of the pure elements. However, efforts are underway to develop new lattice stabilities of the pure elements that are valid down to 0 K and within this context it is highly desirable that the descriptions of the molar volume are also valid for these temperatures. An overview of these recent developments in CALPHAD modeling will be presented.