INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Seminar

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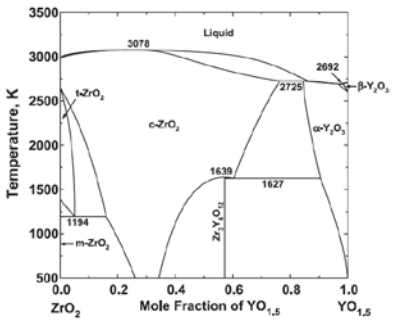
Monday, May 21, 4:30 p.m. ICAMS Seminar room UHW 11/1102

Calphad modelling of oxide systems

Phase diagrams and thermodynamic data for oxide systems are important for applications such as slag metallurgy, refractory ceramics, high temperature superconductors, solid-oxide fuel cells, Li ion batteries, oxidation of alloys and many more. In the modelling of liquid and solid solutions it is usually necessary to take the formal oxidation state (valency) of the constituents into account. For solid solutions the compound energy formalism (CEF) developed by Hillert and co-workers is used very extensively. When ions are introduced into this formalism it is usually found there is not a one-to-one correspondence between model compounds and real compounds (which could in principle be synthesised). This makes the CEF sometimes quite tricky to handle for ionic solutions. For the purpose of modelling phase diagrams and thermodynamic properties it is only necessary to take the major defects into account, and many solids can be modelled as stoichiometric or partially stoichiometric compounds. However, when modelling diffusion it also becomes necessary to consider some of the minor defects. This talk will focus on the modelling of ionic solid solutions using the compound energy formalism.



M. Chen, B. Hallstedt, L.J. Gauckler, Solid State Ionics, 170 (2004) 255–74