The CALPHAD (CALculation of PHAse Diagrams) approach applied to the fluoride compounds

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Phase diagrams are visual representations of the state of a material as a function of temperature, pressure and concentrations of the constituent components. They are used in materials research and engineering to alloy design, development, processing and basic understanding. Industrial processes require also reliable thermodynamic data. The CALPHAD approach is based on the fact that a phase diagram is a manifestation of equilibria based on the total Gibbs energy minimization of a system. The aim of this method is to develop consistent thermochemical representation for the phase equilibria and thermodynamics properties of all the phases (as well stoichiometric compounds, solution than vapor species) of a system utilizing all available informations. It permits prediction of properties of multicomponent systems from those of binary and ternary subsystems, critical assessment of data and their incorporation into self-consistent databases. Databanks are then used for calculations to improve understanding of various industrial and technological processes.
In this lecture, we would like to present the CALPHAD methodology (Figure 1) and give some examples with fluoride compounds.

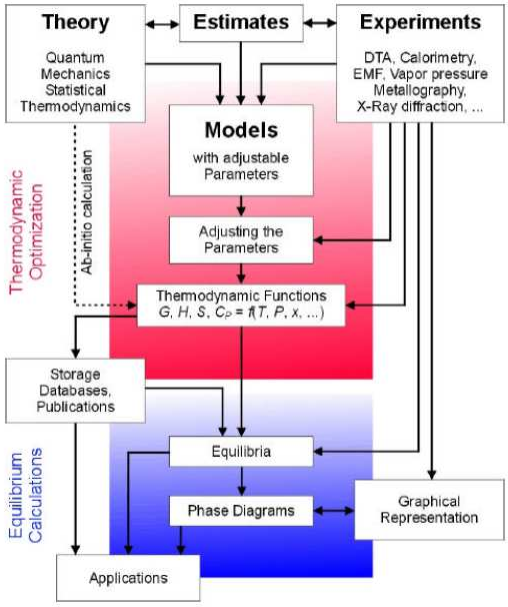

Figure 1: Flowchart of the CALPAHD method after Zinkevich [1].

References

1. M. Zinkevich, *Computational Thermodynamics: Learning, Doing and Using*, Presentation at the International Max Planck Research School for Advanced Materials: Theoritical and Computational Materials Science, 1st Summer School, Stuttgart, Germany, 2003