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 design and develope alloys, devise processing methodologies and enhance basic understanding of materials behavior. The CALPHAD approach is based on the fundamental axiom 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 (e.g., stoichiometric compounds, solutions, liquid and vapor species) of a system utilizing all available information. Also, CALPHAD methodology permits extrapolation of the properties of multicomponent systems from those of binary and ternary subsystems that are already critically assessed and incorporationed into self-consistent databases. Therefore, these databases are extremely useful for preforming calculations to improve understanding of various industrial and technological processes.
In this lecture, we will present the CALPHAD methodology (Figure 1), discuss the thermodynamic databases and data used, and give several key fluoride compounds examples.

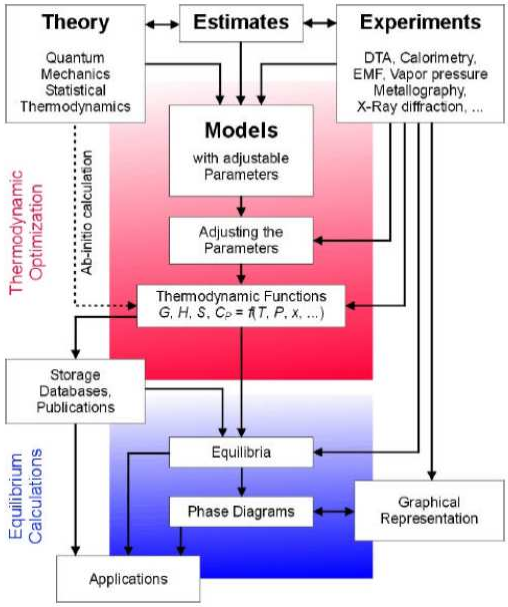

Figure 1: Flowchart of the CALPAHD method after Zinkevich [1].

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