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Bo SUNDMAN et al.

KTH (Sweden) and CEA-INSTN (France)

**The Use of Computational Thermodynamics to Predict
Properties of Multicomponent Materials for Nuclear
Applications**

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The Use of Computational Thermodynamics to Predict Properties of Multicomponent Materials for Nuclear Applications

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Computational Thermodynamics is based on physically realistic models to describe metallic and oxide crystalline phases as well as the liquid and the gas in a consistent manner [1]. The models are used to assess experimental and theoretical data for many different materials and several thermodynamic databases has been developed for steels, ceramics, semiconductor materials as well as materials for nuclear applications.

Within CEA a long term work is ongoing to develop a database for the properties of nuclear fuels and structural materials [2].

An overview of the modeling technique will be given and several examples of the application of the database to different problems, both for traditional phase diagram calculations and its use in simulating phase transformations. The following diagrams (Fig. 1, Fig. 2 and Fig.3) show calculations in the U-Pu-O system.

Fig. 1 : U-Pu-O phase diagram at 1273°K.

Fig. 2 : U-Pu-O phase diagram at 673°K showing the miscibility gap in the MO₂ phase together with experimental data.

Fig. 3 : Oxygen chemical potentials at different temperatures and varying oxygen content for systems with Pu/u ratios around 0.3, together with experimental data.

References

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- [2] C. Guéneau, N. Dupin, B. Sundman, C. Martial, J.-C. Dumas, S. Gossé, S. Chatain, F. De Bruycker, D. Manar, R.J.M. Konings, Thermodynamic modeling of advanced oxide and carbide nuclear fuels: description of the U-Pu-O-C systems. J. Nucl Mater. 419 (2011) 145

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Abstract

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Literature:

- ▶ Nigel Saunders and Peter Miodownik, *Calphad*, Pergamon Materials Series, Vol 1 (1998)
- ▶ Mats Hillert: *Phase Equilibria, Phase Diagrams and Phase Transformations*, 2nd edition, Cambridge (2008).
- ▶ Leo Lukas, Suzana Fries and Bo Sundman, *Computational Thermodynamics*, Cambridge (2007).

Classical Thermodynamics

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These laws, and some trivial mathematics, makes it possible to define a number of additional properties like internal energy, U , entropy, S , Gibbs energy, G etc. These are not observables but can be used to derive strict mathematical relations between many properties.

Properties derived from the Gibbs energy

$$S = - \left(\frac{\partial G}{\partial T} \right)_{P, N_i}$$

$$H = G - TS$$

$$V = \left(\frac{\partial G}{\partial P} \right)_{T, N_i}$$

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$$C_P = -T \left(\frac{\partial^2 G}{\partial T^2} \right)_{P, N_i}$$

$$\alpha = \frac{1}{V} \left(\frac{\partial^2 G}{\partial P \partial T} \right)_{N_i}$$

$$\kappa = -\frac{1}{V} \left(\frac{\partial^2 G}{\partial P^2} \right)_{T, N_i}$$

Computational Thermodynamics: Central part of science

Computational Thermodynamics: Models 1

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For the configurational entropy one must take into account the formation of molecules in a gas phase, crystalline sites in solids, charge transfer between elements, clusters etc. In many cases it is necessary to introduce more constituents of the phases than just the components.

Computational Thermodynamics: Models 2

Most materials consists of several crystalline phases with different structure and properties. The material often interact with other phases like gas and liquids.

The Gibbs energy is an extensive property and it is possible to model each phase separately:

$$G = \sum_{\alpha} N^{\alpha} G_m^{\alpha}(T, P, y_i)$$

where N^{α} is the number of moles and G_m^{α} is the molar Gibbs energy of of the phase α .

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Computational Thermodynamics: Models 3

In a gas phase the molecules like H_2 , H_2O , O_2 etc. are the constituents. The mole fraction of component i in the gas is

$$x_i^{\text{gas}} = \frac{\sum_j b_{ij} y_j^{\text{gas}}}{\sum_k \sum_j b_{kj} y_j^{\text{gas}}}$$

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In a crystalline phase one may have several sublattices with are preferred by different elements.

$$x_i^{\alpha} = \frac{\sum_s a_s \sum_j b_{ij} y_j^{(s),\alpha}}{\sum_s a_s \sum_k \sum_j b_{kj} y_j^{(s),\alpha}}$$

where a_s is the number of sites on sublattice s , b_{ij} is the stoichiometric factor and $y_j^{(s)}$ is the fraction of constituent i on sublattice s .

Computational Thermodynamics: Models 4

The figures below represent three crystalline structures, B1, D8_b and D0₃ which require sublattices to be modelled.

The Compound Energy Formalism (CEF) assumes random mixing of the constituents on each sublattice which gives the configurational entropy as

$$^{\text{cfg}}S_m = \sum_s a_s \sum_i y_i^{(s)} \ln(y_i^{(s)})$$

Computational Thermodynamics: Models 5

The *end member* is an important concept in CEF defining one specific constituent in each sublattice. This defines a compound and the surface of reference for the phase:

$$^{\text{srf}}G_m = \sum_I \prod_{i_l} y_i^{(s)} \circ G_I$$

where I has one constituent i in each sublattice s and $\circ G_I$ is the Gibbs energy of formation of this compound from the reference states of the elements, depending only on T and P .

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In order to represent the interaction energy between the constituents in sublattices there is an excess Gibbs energy:

$$^E G_m = \sum_J \prod_{j_J} y_j^{(s)} L_J$$

where J has one or more constituents in each sublattice and L_J describe the properties of real phases.

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Phase fractions in MOX

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As the Gibbs energy curves are modelled outside the stable range of the phases it is possible to calculate metastable states.

Computational Thermodynamics: Software 3

The diagrams below show the modelled Gibbs energy functions for two phases in a binary system at 3 different temperatures.

In two-phase regions the *common tangents* to the Gibbs energy curves gives the most stable state.

The vertical dashed lines indicate the compositions of the phases for the common tangents.

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The diagrams below show the modelled Gibbs energy functions for two phases in a binary system at 3 different temperatures.

The solubility lines in the phase diagram are obtained by joining the points of the common tangents at varying temperatures.

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Some model parameters, like the description of pure elements, must not be changed because that would make it impossible to combine assessments.

Computational Thermodynamics: Assessment 1

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At CEA there is an ongoing project to develop the *fuelbase database* for nuclear fuels, fission products, and structural materials.

In recent assessments results from DFT calculations have been included for the formation of defects and metastable compounds.

Diagrams calculated from fuelbase

Cr-Fe

CaO-SiO₂

O-U

O-U

Cr-Fe-Ni at 1073 K

Al₂O₃-CaO-SiO₂ at 1673 K

Isothermal section of Am-O-Pu at 1273 K

Modelling ionic systems 1

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In crystalline phases vacancies are often needed to describe defects or deviations from stoichiometry.

A simple case is wustite (periclas, halite) with a B1 structure modelled as

Modelling ionic systems 2

The C1 structure, CaF_2 , is the same structure as MO_2 in nuclear fuels modelled with several metallic valencies and defects on the oxygen sublattice and interstitial oxygen. The shaded plane is the neutral combination of defects.

The end members can be drawn in different ways, either varying occupancy of the oxygen sublattices at constant valency of U (top square prism) or varying U valencies at constant occupancy of the oxygen sublattices (bottom triangular prism).

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For the U-Pu-O system the model is:

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$${}^\circ G_{3:\text{O}:\text{V}} + {}^\circ G_{5:\text{O}:\text{V}} - 2 {}^\circ G_{4:\text{O}:\text{V}}$$

The Frenkel defects forming interstitial oxygen is given by

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- ▶ Thermodynamics provide information on the gradients in chemical potential driving the diffusion in phase transformations.
- ▶ The thermodynamic factor, the matrix with the second derivatives of the Gibbs energy, is needed to evaluate diffusion coefficients.

Conclusions

There are many factors which must be modelled and determined experimentally in order to understand the behaviour of multicomponent materials.

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With an assessed thermodynamic database it is easy to calculate the set of stable set of phases, their amount and composition and the chemical potentials of the components for the varying external conditions.

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There are many factors which must be modelled and determined experimentally in order to understand the behaviour of multicomponent materials.

With an assessed thermodynamic database it is easy to calculate the set of stable set of phases, their amount and composition and the chemical potentials of the components for the varying external conditions.

This is a great help to select critical experimental work and to use in software for simulation of phase transformations.

Thanks

for listening