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

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KTH (Sweden) and CEA-INSTM (France)
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.

![U-Pu-O phase diagram at 1273°K.](image1)

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

![U-Pu-O phase diagram at 673°K showing the miscibility gap in the MO\(_2\) phase together with experimental data.](image2)

**Fig. 2 :** U-Pu-O phase diagram at 673°K showing the miscibility gap in the MO\(_2\) 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.

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December 5, 2012
Abstract

Computational Thermodynamics is based on physically realistic models to describe metallic and oxide crystalline phases as well as the liquid and gas in a consistent manner. 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. An overview of the modelling technique will be given and several examples of the application of the database to different problems.
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- Computational Thermodynamics (CT, Calphad)
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- Leo Lukas, Suzana Fries and Bo Sundman, *Computational Thermodynamics*, Cambridge (2007).
Classical Thermodynamics

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It is founded on two simple laws for macroscopic systems:

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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

\[ S = - \left( \frac{\partial G}{\partial T} \right)_{P, N_i} \]
\[ H = G - TS \]
\[ V = \left( \frac{\partial G}{\partial P} \right)_{T, N_i} \]
\[ \mu_i = \left( \frac{\partial G}{\partial N_i} \right)_{T, P, N_j \neq i} \]
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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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- the configurational entropy is very important.

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 consist 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 \( N_\alpha \) is the number of moles and \( G_m^\alpha \) is the molar Gibbs energy of the phase \( \alpha \).
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\[ G = \sum_{\alpha} \xi_\alpha G_m(\alpha, T, P, y_i) \]

where \( \xi_\alpha \) is the number of moles and \( G_m^\alpha \) is the molar Gibbs energy of the phase \( \alpha \). The molar Gibbs energy is written as a function of the constituent fractions, \( y_i \), to model the configuration of the phase. In this way each phase can be modelled independently. The equilibrium is found by minimizing the total Gibbs energy for the given set of external conditions.
In a gas phase the molecules like H$_2$, H$_2$O, 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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where $b_{ij}$ is the stoichiometric ratio of component $i$ in $j$. 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 $s$. 
The figures below represent three crystalline structures, B1, D8\(_b\) and D0\(_3\) 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:

\[
s_{\text{rf}} G_m = \sum_{l} \prod_{i_l} y_i^{(s)} \circ G_I
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where \( l \) 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:

\[ E \ G_m = \sum_J \prod_{j_J} y_{j_J}^{(s)} L_J \]

where \( J \) has one or more constituents in each sublattice and \( L_J \) describe the properties of real phases.
Computational Thermodynamics: Software 1

There are several commercial software for equilibrium calculations and they offer slightly different ways to control a system. The simplest way is to specify $T$, $P$ and the amount of all components.
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![Graph showing oxygen potentials in UO₂](image)

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Oxygen potentials in UO$_2$

The heat capacity of UO$_2$
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When two or more conditions are allowed to vary the software will calculate a *phase diagram* where the lines separate regions with different sets of stable phases.

The leftmost diagram is the O-Zr phase diagram, the middle diagram is an isothermal section at 473 K of the O-Pu-U phase diagram and the rightmost an isopleth section of the C-O-Pu-U system.
The diagrams below show the modelled Gibbs energy functions for two phases in a binary system at 3 different temperatures.
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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.
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 solubility lines in the phase diagram are obtained by joining the points of the common tangents at varying temperatures.
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By combining several binary and ternary assessments one can construct multicomponent databases. Normally adjustments are needed to obtain correct multicomponent extrapolations. 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

Critical review of the literature data
- Phase diagrams
- Thermodynamic data
- Crystalline data

Choice of the model
- Sublattice model for each phase
- Variables to be optimized

Determination of thermodynamic data
- Phase diagram (DTA, heat treatment ...) Activities (EMF, KCMS, TGA ...)
- Enthalpies, heat capacities (calorimetry, ab-initio)

Selection of experimental data

Selection of the variables for the optimization

OPTIMIZATION

If the fit is not good

Database \( G \text{ phase} = f (T, x, P) \)

If the fit is good

If the fit is not good

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Computational Thermodynamics: Assessment 2

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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

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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The difficulty with modelling oxides is the charge transfer. Normally each oxygen atom will take two electrons from the metallic atoms, some with multiple valencies, and a separate charge balance is needed for the equilibrium. In crystalline phases vacancies are often needed to describe defects or deviations from stoichiometry.

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

$$(\text{Fe}^{+2}, \text{Fe}^{+3}, \text{Va})_1(\text{O}^{-2})_1$$
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:

\[(U^{+3}, U^{+4}, U^{+5}, Pu^{+3}, Pu^{+4})_1(O^{-2}, Va)_2(O^{-2}, Va)_1\]
Modelling ionic systems 2

Most of the end members of the UO\(_2\) model have a net charge and cannot be measured or even calculated by DFT. But one can make neutral combinations related to the formation of compounds.

The reaction for electronic defects is
\[
2U^{4+} = U^{3+} + U^{5+}
\]
and expressed by the difference of 3 end members
\[
\deg{G_3:O:V} + \deg{G_5:O:V} - 2 \deg{G_4:O:V}
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\[ \circ G_{3:O:V} + \circ G_{5:O:V} - 2 \circ G_{4:O:V} \]

The Frenkel defects forming interstitial oxygen is given by

\[ \circ G_{4:O:O} + \circ G_{4:V:O} - 2 \circ G_{4:O:V} \]
Summary

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▶ Thermodynamics provide information on the gradients in chemical potential driving the diffusion in phase transformations.
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- It is also possible to include kinetic data like mobilities in the databases but that require additional assessment work.
- The thermodynamic models can be extrapolated to metastable states and calculate the driving forces for precipitation of new phases.
- 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.

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

for listening