“Fundamentals of Thermodynamic Modelling of Materials”

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PROFESSOR & TOPIC

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Computational Thermodynamics (CT)

[01001]

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Computational Thermodynamics
An overview

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A puzzle to be solved till the end of the week:
to which lecture is each one of the images related?
Computational Thermodynamics
An overview

- Name created by Bo Sundman in order to label KTH department where Kinetic and Thermodynamic databases for technical materials were being created using CALPHAD.

- Nowadays the term is used in a generalized way, even when CALPHAD is not used.

The big advantage is that the label, now incorporates, for example, enthalpies of formation calculated by theoretical physicists using Density Functional Theory. Even if the objective is not to use the results in CALPHAD databases, the contribution for CALPHAD is done.
Computational Thermodynamics
What is it CALPHAD?

It is not a software!

It is a method!

Gibbs energies for all the stable phases of a system are described by parametric models. These parameters are obtained in such a way that the Gibbs energy and its derivatives reproduce the experimental corresponding value at its best.

When this is done, by Gibbs energy minimization the phase diagram can be calculated! CALculated PHAse Diagrams

Big advantages: interpolations and extrapolations can be done. Less experiments are need. Even some antecipation of higher order systems can be done!

Interpolations are so good as the description...Extrapolations too and they are not trully predictable.
If there is a ternary compound that is not in the description it can not be guessed by the extrapolation from the binaries.

Computational Thermodynamics
The CALPHAD method.

\[
\begin{align*}
\text{unary:} & \quad G = \sum_i x_i G_i^0 + RT \sum_i x_i \ln x_i + G^\infty \\
\text{binary:} & \quad \text{Assessment: } G^\infty \\
\text{ternary:} & \quad \text{Extrapolation: } \left( \sum_i G_i^0 \right) + \text{Assessment: } G^\infty \\
\text{quaternary:} & \quad \text{Extrapolation: } \left( \sum_i G_i^0 + \sum_j G_j^0 \right) + \text{Assessment: } G^\infty \\
\end{align*}
\]

From Ursula Kattner
Computational Thermodynamics
The CALPHAD method.

1-Needs Gibbs energy databases.

2-Needs a Gibbs energy minimizer.

Only to say CALPHAD is not enough, one should say which database is used! And they are several, even for the same material!!

Minimizers are also several, and if they use the same database, the calculated results should be the same...
Computational Thermodynamics

For what?

Even in the case one has a good Gibbs energy database, one still do not have the very relevant feature of materials properties: the microstructure.

A microstructure pattern is not like a state variable. It depends on the processes!

Then simulations are necessary. Phase Field is a powerful method.

They are more realistic if they have some realistic information to where the whole system evolves.

To know the equilibrium thermodynamics is them a part of that simulations.

Computational Thermodynamics

Microstructure related quantities

Even a material made by a single element can present different microstructures:
- single crystal
- polycrystalline
- nanograins

All that results in different properties even if the chemistry is the same.

For the two last items there are interfaces!!
This is usually not in CALPHAD databases.
Computational Thermodynamics
Being truly predictive...the big challenge. This school gives you some hints...

First-principles domain, usually Zero K

CALPHAD starts at 298.15

(All possible combinations of periodic table)

Connecting CALPHAD and DFT

298.15 K
CALPHAD START

0.00 K
DFT START

All possible combinations of periodic table

All crystal structures
Connecting CALPHAD and DFT

At any
Adding pressure

0.00 K
DFT START

298.15 K
CALPHAD START
At any

Arranging the material in the space

The microstructures can then be more realistic simulated.
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Winter School : « Fundamentals of Thermodynamic Modelling of Materials »