“ Fundamentals of Thermodynamic Modelling of Materials ”

November 15-19, 2010
INSTN – CEA Saclay, France

PROFESSOR & TOPIC

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*Computational
Thermodynamics(CT)*

[01001]

Organized by

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Computational Thermodynamics

An overview

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15 - 19 novembre • INSTN, Saclay, France

Winter School : « Fundamentals of Thermodynamic Modelling of Materials »

Computational Thermodynamics

An overview

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

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Computational Thermodynamics

An overview

	Monday 15	Tuesday 16	Wednesday 17	Thursday 18	Friday 19
9.00	Computational	Thermodynamics from	Thermodynamic	Simulation of the	Magnetic models
9.15	Thermodynamics (CT)	lattice dynamics w DFT	assessments	thermodynamics of	for CT
9.30	Suzana Fries	Stefano Baroni	Nathalie Dupin	surfaces and interfaces	
9.45	Application of CT	Potential energy	Experimental data	Julian Gale	Pavel Korzhavyi
10.00	for superalloys	surfaces	for assessments	coffee	coffee
10.15	Roger Reed	Julian Gale	Jean-Marc Joubert		
10.30	coffee	coffee	coffee	Multicomponent	High pressure models
10.45				diffusion simulation	for CT
11.00	Thermodynamic	Monte Carlo simulation	Theoretical data	Lars Hoglund	Michael Jacobs
11.15	modelling	Frederic Soisson	for assessments	Phase field	Summary and
11.30	Bo Sundman		Pavel Korzhavyi	simulations	evaluation
11.45	Beyond standard DFT	Monte Carlo for spin	Extrapolations from		
12.00		crossover compounds	thermodynamic models	Alphonse Finel	All
12.15	Georg Kresse	Jorge Linares	Suzana Fries		
12.30					
12.45					
13.00	Lunch	Lunch	Lunch	Lunch	Lunch
13.15					
13.30					
13.45					
14.00					
14.15	Calculation of	Monte Carlo	Molecular and	Phase field and	School dinner: Tuesday evening
14.30	thermodynamic	simulations	lattice dynamics	diffusion simulations	
14.45	properties		simulations		
15.00					
15.15	Ab initio calculations	Ab initio calculations	Thermodynamic	coffee	
15.30	at 0 K	at finite temperatures	assessments		
15.45	coffee	coffee	coffee		
16.00					
16.15					
16.30	Ab initio calculations	Ab initio calculations	Thermodynamic	Phase field and	
16.45	at 0 K	at finite temperatures	assessments	diffusion simulations	
17.00					
17.15					

ICAMS

RUB

Computational Thermodynamics

What is it?

- 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.

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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 needed. Even some anticipation of higher order systems can be done!

Interpolations are so good as the description...Extrapolations too and they are not truly 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.

• From Ursula Kattner

Computational Thermodynamics

The CALPHAD method.

From Bo Sundman

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 calculate results should be the same...

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For what?

Even in the case one has a good Gibbs energy database, one still don't 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 then a part of that simulations.

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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.

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Being trully predictive...the big challenge.
This school gives you some hints...

Connecting CALPHAD and DFT

Connecting CALPHAD and DFT

The microstructures can then be more realistic simulated

The microstructures can then be more realistic simulated

Computational Thermodynamics

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9.15	Suzana Fries	Stefano Baroni	Nathalie Dupin		
9.30	Application of CT for superalloys	Potential energy surfaces	Experimental data for assessments	Julian Gale	Pavel Korzhavyi
9.45	Roger Reed	Julian Gale	Jean-Marc Joubert	coffee	coffee
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11.00	Thermodynamic modelling	Monte Carlo simulation	Theoretical data for assessments	Multicomponent diffusion simulation	High pressure models for CT
11.15	Bo Sundman	Frederic Soisson	Pavel Korzhavyi	Lars Hoglund	Michael Jacobs
11.30	Beyond standard DFT	Monte Carlo for spin crossover compounds	Extrapolations from thermodynamic models	Phase field simulations	Summary and evaluation
11.45	Georg Kresse	Jorge Linares	Suzana Fries	Alphonse Finel	All
12.00					
12.15					
12.30					
12.45					
13.00	Lunch	Lunch	Lunch	Lunch	Lunch
13.15					
13.30					
13.45					
14.00					
14.15	Calculation of thermodynamic properties	Monte Carlo simulations	Molecular and lattice dynamics simulations	Phase field and diffusion simulations	School dinner: Tuesday evening
14.30					
14.45					
15.00					
15.15					
15.30	Ab initio calculations at 0 K	Ab initio calculations at finite temperatures	Thermodynamic assessments	coffee	
15.45	coffee	coffee	coffee		
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