Phase Equilibria and Transformations - Presentation of various software approaches

4 - 6 June 2013
European Training Course
Maria-Laach

Deutsche Gesellschaft
für Materialkunde e.V.
Senckenberganlage 10
60325 Frankfurt
Germany

Scope / Speakers

The development and optimisation of new materials for applications under enhanced and complex service conditions require new instruments for the treatment of transformations. They have to be based on fundamental principles in order to provide predictability. Empirical approaches cannot meet these requirements.

In practice materials are multi-component systems. Their phase equilibria can only be obtained using numerical techniques. This gave rise to the computational thermodynamics which is based on a description of the thermodynamic functions by appropriate modelling. The parameters of these functions are obtained from experimental data by optimization methods. At present thermodynamic databases are available for various classes of materials representing a valuable tool for materials development and for the solution of complex technological problems. The calculation of stable and metastable phase equilibria as function of temperature and composition provides the basis for determining the effect of alloying elements on the precipitation behaviour. Chemical reactions can be calculated under various boundary conditions yielding the input for process simulation.

The computer simulation of phase transformations, based upon multi-component thermodynamics, offers an excellent tool for treating the kinetics of microstructure formation. This includes the morphological evolution during transitions, the prediction of precipitation sequences of stable and meta-stable phases and microstructural long term stability. Since data on true thermodynamic driving forces are provided by the thermodynamic software, the required kinetic data are reduced to the mobilities of the elements in the various structures. These are available for many substances and phases.
At present there exist three different approaches focusing on different aspects: (a) the sharp interface concept with local equilibrium at the moving boundary (DICTRA), (b) the phase field method with a diffuse interface allowing for a treatment of morphological evolutions like dendritic solidification (MICRESS), (c) the meanfield treatment of multi-component, multi-phase precipitation using the concept of maximum rate of entropy production (Onsager's extremum principle), including finite interface mobilities and large deviations from local equilibrium (MatCalc).

It is the aim of this seminar
- to present these approaches in detail,
- to show their excellent predictive capability,
- to demonstrate how to work with the software.

This will be done interactively by particular case studies.

The seminar addresses materials engineers and scientists in research and development departments in industry and at Universities.

Chairman of the seminar is **Prof. Dr. G. Inden**, retired from Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf.

Further speakers are:

Dr. M. Apel
Dr. B. Böttger
RWTH Aachen, Access e.V., Germany

Prof. Dr. K. Hack
GTT-Technologies, Herzogenrath

Speakers / General Information

Dr. Å. Jansson
Thermo-Calc Software AB, Stockholm, Sweden

Prof. Dr. E. Kozeschnik
Institute of Materials Science and Technology, Vienna University of Technology, Austria

Prof. Dr. R. Schmid-Fetzer
Clausthal University of Technology, Institute of Metallurgy

The seminar takes place in the Seehotel Maria Laach situated 15 km west of Koblenz. It is overlooking the wide round of the largest Eifel maar, a volcano that has become extinct about 10000 years ago and that now forms a lovely lake surrounded by low mountains and isolated forests. Next to the Seehotel is the 900 year old monastry Maria Laach, a holy place for contemplation and meditation.

The Seehotel offers state-of-the-art teaching and learning facilities for conferences and seminars in the immediate vicinity of a healing bath with strengthening effect on everybody. Detailed information is available on the Seehotel website: www.seehotel-maria-laach.de

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Fee for Members of the DGM:
Personal members or 1 non-member from a member institute / member company: 1.550,- EURO

Participation fee
including full accomodation:
1.650,- EURO

The fee includes:
- Attendance of the seminar sessions
- Comprehensive handouts
- Refreshments during the sessions
- Lunch and dinner
- Accomodation (2 nights/4-6 June 2013))

Together with the registration, accomodation and breakfast in the Seehotel will be firmly arranged. This allows to extend communication and networking during the evenings.

Cancellation policy:
Any cancellation is subject to a cancellation fee of 50% of the fees involved. After 7 Mai the entire fee is due. Substitution is possible at any time.

NEW

DGM

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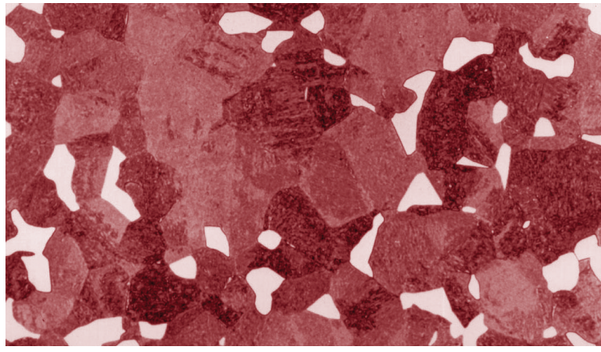

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Max-Planck-Institut für
Eisenforschung, Düsseldorf

Deutsche Gesellschaft
für Materialkunde e.V.

www.dgm.de

Chairman of the seminar

Prof. Dr.
G. Inden

Tuesday

8:30 G. Inden
Computational Thermodynamics
Reminder of thermodynamic principles; Databases; Equilibria

Presentation of different thermodynamic software

Å. Jansson
9:15 **Software: Thermo-Calc**
Calculation of stable and metastable equilibria in multi-component systems, phase diagrams; Scheil solidification; Thermodynamic databases

10:15 Coffee break

10:30 K. Hack
Software: FactSage, ChemApp, ChemSheet, SimuSage, SolKin
Thermodynamic properties, stoichiometric reactions, complex equilibria and phase diagrams; The concept of local equilibrium in process simulation

11:30 R. Schmidt-Fetzer
Software: Pandat
Calculation of phase equilibria and thermodynamic properties in multi-component systems

12:30 Lunch

Practical demonstration of thermodynamic software

13:30 Å. Jansson, G. Inden
Thermo-Calc

15:00 K. Hack
Factsage, ChemApp, Chemsheet, Simusage

16:30 Coffee break

17:00 R. Schmidt-Fetzer
Pandat

18:30 **Discussion**

19:15 Dinner and individual demonstrations

Wednesday

Presentation of software for phase transformations

8:30 G. Inden
Introduction into the software DICTRA
Sharp interface; Concept of mobility; Local equilibrium (LE); local equilibrium no partitioning (LENP); para-equilibrium (PARA)

9:45 M. Apel
Concept of a diffuse interface (MICRESS)
Phase transformation as a free boundary problem; solid state transformations, solidification, grain growth and ripening, nucleation

11:00 Coffee break

11:15 E. Kozeschnik
Predictive modeling of complex precipitation systems (MatCalc)
Kinetics of precipitation in multi-component; multi-particle and multi-phase systems; Interfacial energy modeling; Evolution of precipitate populations at dislocations and grain boundaries; Precipitation strengthening; Coupled treatment of precipitation and deformation

12:30 Lunch

Practical demonstration of kinetic software

13:30 G. Inden, Å. Jansson
Practical demonstration of DICTRA simulations
Precipitation in various geometries, simultaneous reactions (multi-cell treatment); various cell boundary conditions (e.g. carburisation)

15:00 E. Kozeschnik
Practical demonstration of MatCalc simulations
Treatment of typical problems of precipitation using GUI and command files, discussion of nucleation parameters and thermodynamic inputs

16:30 Coffee break

Wednesday

17:00 B. Böttger
Practical demonstration of MICRESS simulations
Microstructure variation as function of alloy composition and processing parameters, evaluation of results

18:30 **Discussion**

19:15 Dinner and individual demonstrations

Thursday

Practical demonstration of kinetic software

8:30 Å. Jansson
TC-PRISMA
concurrent nucleation; growth and coarsening Langer-Schwartz theory; Kampmann-Wagner numerical approach

9:30 R. Schmidt-Fetzer
PanPrecipitation
simultaneous nucleation; growth and coarsening multi-level kinetic models (JMAK, Langer-Schwartz; Kampmann-Wagner); strengthening model

10:30 Coffee break

10:45 M. Apel, G. Inden,E. Kozeschnik
Examples of materials and process development using thermodynamic and kinetic software

12:15 **Concluding remarks**

12:30 End of the seminar

Registration

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☐ DGM-member

DGM-Membership Number

Phone

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