# **Thermodynamics** Computer-Aided

eutsche Gesellschaft ür Materialkunde e.V. enckenberganlage 10 0325 Frankfurt

Scope / Speakers

The properties of materials strongly depend on their microstructure. The microstructure is the result of phase transformations occurring during appropriate heat treatments. Since these treatments are limited in time, stable as well as metastable phases may participate in these reactions. It is thus very important to know about these stable and metastable phase equilibria in the field of materials development and optimization.

In practice materials are multicomponent 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 fun- Institute of Materials Technology ction of temperature and composition provides the basis for determi- Prof. Dr. K. Hack ning the effect of alloying elements on the precipitation behaviour. Similarly, chemical reactions can be calculated under various boundary conditions yielding the input for process simulation. The calculation of equilibria under time dependent conditions leads to reaction paths.

It is the aim of this training course to present the actual status of various software packages for thermodynamic calculations and to Institute of Metallurgy

give a comprehensive and comprehensible overview of the applications. A wide field of materials will be covered, ranging from steels, electronic materials, noble metals, solders and amalgams. Specific examples of industrial applications will be presented. In addition, broad room will be given to live and interactive demonstrations in order to give a good insight into the handling of the different types of software.

The training course addresses to materials research and development departments in industry and at

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

Further speakers are:

Dr. U. Diekmann Metatech GmbH, Kamen

Dr. C. Ernst Deutsche Edelstahlwerke, Witten

Dipl.-Ing. Bronislava Gorr University of Siegen

GTT-Technologies, Herzogenrath

Dr. Å. Jansson

Thermo-Calc Software AB. Stockholm

Prof. Dr. M. Rettenmayr Friedrich-Schiller-University Jena Institute of Materials Science and

Prof. Dr. R. Schmid-Fetzer Clausthal University of Technology

Technology



Seehotel Maria-Laach

# General Information

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 member company: 1.550,- EURO and isolated forests. Next to the Seehotel is the 900 year old mona- The fee includes: stry 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:

For further information please contact: Deutsche Gesellschaft für Materialkunde e.V. Niels Parusel Senckenberganlage 10 60325 Frankfurt Germany

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# Participation fee

including full accomodation: 1.650,- EURO

#### Fee for Members of the DGM:

Personal members or 1 nonmember from a member institute/

- Attendance of the seminar
- · Comprehensive handouts
- Refreshments during the
- Lunch and dinner
- Accomodation (2 nights)

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 15 June the entire fee is due. Substitution is possible at any time.



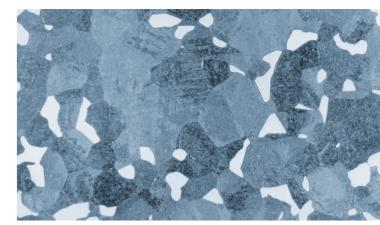
# **DGM Training Courses** and Conferences in 2011

06.0311.03.	Systematische Beurteilung technischer Schadensfälle
10.03.	DFG- und AiF-Fördermittel erfolgreich einwerben
15.0318.03.	Einführung in die Metallkunde für Ingenieure und Techniker
21.0325.03.	Metallkunde für Ingenieure und Techniker
23.0325.03.	Biomaterialien
28.0329.03.	Löten - Grundlagen und Anwendungen
29.0330.03.	Modellierung und Simulation
30.0331.03.	Titan und Titanlegierungen
04.0406.04.	Entstehung, Ermittlung und Bewertung von Eigenspannungen
12.0413.04.	Schweißtechnische Problemfälle
11.0513.05.	Werkstofffragen der Hochtemperatur-Brennstoffzelle (SOFC)
17.0518.05.	Neue Luftfahrt-Werkstoffe
19.0520.05.	Optimierung von Geschäftsabläufen (Workflows)
23.0524.05.	Walzen - Planheit
07.0608.06.	Tribologie
29.0601.07.	Praxis der Bruch- und Oberflächenprüfung
04.0705.07.	Grundlagen der Nanotechnologie
04.0706.07.	Simulation of Phase Transformation
06.0708.07.	Computer-Aided Thermodynamics

18.10.-19.10. Zellulare metallische Werkstoffe

# **European Advanced Training Course**

# **Computer-Aided Thermodynamics**



6-8 July 2011

#### Maria-Laach

Deutsche Gesellschaft für Materialkunde e.V.

Max-Planck-Institut für Eisenforschung, Düsseldorf

www.dgm.de

# Wednesday

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#### **Morning: Arrival**

13:30 G. Inden Welcome

13:40 G. Inden

#### **Computational Thermodynamics**

- Reminder of thermodynamic principles
- Data assessment / Databases / Pure Elements / Alloy systems
- Equilibria

Presentation of different thermodynamic software

14:30 Å. Jansson

#### Software: Thermo-Calc

- Calculation of equilibria in multi-component systems
- 15:45 Coffee break
- 16:15 K. Hack, M. Rettenmayr

#### Software: FactSage, ChemApp, ChemSheet, SimuSage, SolKin

- Thermodynamic properties, stoichiometric reactions, complex equilibria and phase diagrams
- The concept of local equilibrium in process simulation
- 17:30 R. Schmid-Fetzer **Software: Pandat**
- 18:45 End of the 1st day
- 19:00 Dinner, informal get together

# Thursday

#### 8:30 C. Ernst

#### Application of Thermo-Calc in tool steel development

- Stable and metastable equilibria
- Solidification according to Scheil
- Optimisation of chemical composition
- Optimisation of heat treatment temperatures and hot deformation processes
- Comparison between calculation and reality (microstructures)

#### 9:30 M. Rettenmayr

# Computer-aided alloy and process development in the industrial practice

- Development of new amalgams for gas discharge
- Precipitation hardening in noble metal alloy systems
- Exothermic reactions during melting of alloy components
- Phase stability in soft solders
- Estimation of solidification intervals

#### 10:00 M. Rettenmayr

#### Scheil or Lever Rule? - Modeling Solidification Kinetics

- Limits of idealized models
- Physical processes influencing concentration and phase distributions
- Examples: microstructural parameters in binary and ternary Al-alloys
- 10:30 Coffe break

## 11:00 U. Diekmann

## Practical use of JMatPro for the modelling of steel properties

- Phase transitions
- Physical and thermo-physical properties
- Mechanical properties

#### 12:00 Lunch

**Practical demonstrations** 

# Thursday

## 13:00 K. Hack

#### FactSage, ChemApp, ChemSheet, SimuSage

14:30 G. Inden. Å. Jansson Thermo-Calc

- 16:00 Coffee break
- 16:15 R. Schmid-Fetzer **Pandat**
- 17:45 U. Diekmann **JMatPro**
- 19:15 Dinner, informal get together

# Friday

#### 8:30 B. Gorr

## Thermodynamics in the Context of High-Temperature Oxidation of conventional and newly developed alloys

Oxidation of Ni-based superalloys

- Nitridation of Ni-based superalloys
- Oxidation of Co-Re model alloys
- Advantage of the extension of FactSage data-files

# 9:30 R. Schmid-Fetzer, G. Inden, K. Hack

## Calculations on demand - Real world problems raised by participants

- Participants are encouraged to present problems of their field of interest.
- It will be tried to solve these problems in live demonstrations using the available software and databases
- 11:00 Coffee break

#### 11:15 G. Inden

### From equilibrium to the simulation of phase transformations (DICTRA)

- Austenit/ferrite transformation
- Carbide precipitation
- Slow and fast reactions
- Competition between stable and metastable phases

#### 12:15 Short final discussion

12:30 End of the seminar

# **Thermodynamics** Registration

**Computer-Aided**