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 equili- the different types of software. bria 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 a function of temperature and composition provides the basis for determining 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 give a comprehensive and compre-

hensible 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 training course addresses to materials research and development departments in industry and at universities.

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

Further speakers are:

Prof. Dr. Hans-Jürgen Christ Institute of Materials Technology, University of Siegen

Dr. Uwe Diekmann Metatech GmbH, Kamen

Dr. Claudia Ernst Deutsche Edelstahlwerke, Witten

Dr. Rolf Großterlinden ThyssenKrupp Stahl AG, Duisburg

Prof. Dr. Klaus Hack GTT-Technologies, Herzogenrath

Dr. A. Jansson Thermo-Calc Software AB, Stockholm (Schweden)

Prof. Dr. Markus Rettenmayr Friedrich Schiller University Jena

Prof. Dr. Rainer Schmid-Fetzer Technical University of Clausthal, Institute of Metallurgy



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 volcanoe 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: www.seehotel-maria-laach.de

For further information please contact: Deutsche Gesellschaft für Materialkunde e.V. Niels Parusel Senckenberganlage 10 60325 Frankfurt Germany +49-(0)69-75306-757 Phone: +49-(0)69-75306-733 Fax: E-Mail: np@dam.de http://www.dgm.de

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 sessions
- Comprehensive handouts
- Refreshments during the sessions
- Lunch and dinner Accomodation

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 May the entire fee is due. Substitution is possible at any time.

Thermodynamics **Computer-Aided**

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DGM

DGM Training Courses and Conferences in 2010

- 02.03.-05.03. Einführung in die Metallkunde für Ingenieure und Techniker
- 17.03.-18.03. Titan und Titanlegierungen
- 21.03.-26.03. Systematische Beurteilung technischer Schadensfälle
- 22.03.-24.03. Entstehung, Ermittlung und Bewertung von Eigenspannungen
- 25.05.-28.05. Euro Superalloys
- 26.05.-27.05. Pulvermetallurgie
- Computer-Aided Thermodynamics 21.06.-23.06.
- 06.07.-06.07. Fördermittel effizient nutzen
- 26.07.-30.07. Junior Euromat 2010
- 24.08.-26.08. MSE 10 Materials Science and Engineering
- 27.10.-29.10. Cellular Materials - CELLMAT 2010
- 15.11.-17.11. Stranggießen
- 02.12.-03.12. Werkstoffprüfung

European Advanced Training Course

Computer-Aided Thermodynamics



21-23 June 2010

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Maria-Laach

Deutsche Gesellschaft für Materialkunde e.V.

Max-Planck-Institut für Eisenforschung, Düsseldorf

www.dgm.de

Monday

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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 / Allov systems
- Equilibria

Presentation of different thermodynamic software

14:30 A. Jansson

Software: Thermo-Calc

- Calculation of equilibria in multi-component systems
- Solidification reaction according to Scheil
- Graphical facilities for representation
- 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
- 19:00 Dinner, informal get together

Tuesday

Examples of industrial application of computational tools

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. Rettenmavr

Computer-aided alloy and process development in the industrial practice

- Development of new amalgams for gas discharge lamps
- 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. Rettenmavr

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 Coffee break
- 10:45 R. Großterlinden

User-defined application of thermodynamic software

The concept of Steel Map and its realisation Applications:

- Effect of pre-heating temperature on the effect of micro-alloying elements in steels with respect to grain growth and toughness
- Effect of traces of Ti on the solubility of Nb(C,N)

Tuesday

Bake Hardening potential of steels

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Interplay between Ti4S2C2 and TiS in IF-steels

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- The role of thermodynamic conditions in the modelling of microstructure formation
- Effect of C-content on the yield point of steels at higher temperatures
- Thermodynamic calculations: Cp, H and transformation enthalpy of super-heated or super-cooled states
- 11:45 U. Diekmann

Practical use of JMatPro for the modelling of steel properties

- Phase transitions
- Physical and thermo-physical properties
- Mechanical properties
- 12:30 Lunch

Practical demonstrations

- 13:30 K. Hack FactSage, ChemApp, ChemSheet, SimuSage
- 14:45 G. Inden, A. Jansson Thermo-Calo
- 16:00 Coffee break

16:15 A. Jansson Precipitation Simulation in Multicomponent Alloy Systems DICTRA news

- 17:00 R. Schmid-Fetzer Pandat
- 18:15 U. Diekmann **JMatPro**
- 19:15 Dinner, informal get together

Wednesday

Further examples of software applications

8:30 H.-J. Christ

Internal high temperature corrosion processes Combination of diffusion and local equilibrium calculations

- Carburisation of Ni-Cr alloys
- Carburisation of austenitic steels
- Internal nitridation of Ni model alloys
- Internal nitridation of Ni-based superalloys

10:00 Coffee break

10:20 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 all of the available software and databases

11:20 G. Inden

From equilibrium to the simulation of phase transformations (DICTRA)

- Austenite/ferrite transformation
- Carbide precipitation
- Slow and fast reactions
- Competition between stable and metastable phases
- 12:15 Final discussion
- 12:30 End of the seminar

Computer-Aided Registration

Thermodynamics

20. 23 21 -Euro Mar