Transformation Phase of Simulation

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

Scope / Speakers

The development and optimisation It is the aim of this seminar 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.

The computer simulation of phase transformation, based upon multicomponent 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 metastable phases and microstructural long term stability. Reliable thermodynamic data are available for a multitude of materials. Since data on true thermodynamic driving forces are available, the kinetic data are reduced to the mobilities of the elements in the various structures. They are also 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 multicomponent, multiphase precipitation using the concept of maximum entropy production (Onsager's extremum principle), including finite interface mobilities and large deviations from local equilibrium (MatCalc)

- to present these approaches in
- to show their excellent predictive capability.
- to demonstrate how to work with the software.

This will be done interactively by particular case studies which include steels, Ni-base alloys, Al-alloys.

The seminar addresses materials engineers and scientists in research and development de-partments 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:

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

Dr. Å. Jansson

Thermo-Calc Software AB. Stockholm, Sweden

Prof. Dr. E. Kozeschnik

Institute of Materials Science and Technology, Vienna University of Technology, Austria



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 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

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

Phone: +49-(0)69-75306-757 +49-(0)69-75306-733 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/ member company: 1.550,- EURO

The fee includes:

- · Attendance of the seminar sessions
- 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.

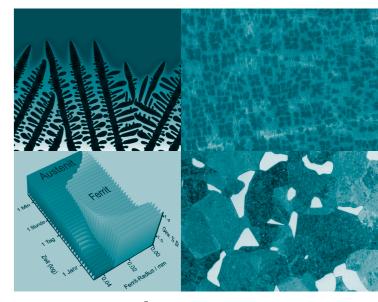
Cancellation policy:

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

European Advanced Training Course

Simulation of Phase Transformation



4-6 July 2011

Maria-Laach

Deutsche Gesellschaft für Materialkunde e.V.

Max-Planck-Institut für Eisenforschung, Düsseldorf

www.dgm.de

Monday

Morning: Arrival

13:30 G. Inden Welcome

13:40 G. Inden

Introduction to new approaches

Failure of empirical approaches Unexpected reactions: effect of alloying elements, role of trace elements, competition between stable and metastable phases

Conceptual options

14:30 G. Inden

Concept of a sharp phase boundary (DICTRA)

Local equilibrium at moving interfaces (LE), local equilibrium no partitioning (LENP), para-equilibrium (PE), fast and slow reactions

- 15:30 Coffee break
- 16:00 M. Apel

Concept of diffuse interface (MICRESS)

Phase transformation as a free boundary problem; dendritic, eutectic and peritectic solidification, solid state transformations, grain growth and ripening, nucleation

17:00 E. Kozeschnik

Concept of maximum rate of Gibbs Energy dissipation (MatCalc)

Precipitation kinetics of spherical particles in multicomponent multi-particle and multi-phase systems. Evolution equations in the case of finite mobility of phase boundaries. Estimation of interfacial energies.

18:00 Å. Jansson

Diffusion in multicomponent systems, kinetic

Concept of mobility, up-hill diffusion, data assessment

19:00 End of day one

19:15 Dinner, informal get together, individual discussions

Tuesday

Software Aspects

8:30 Å. Jansson

Introduction into the software DICTRA

Introduction into the command structure, definition of problems, facilities for graphical representations

9:30 E. Kozeschnik

Introduction into the software MatCalc

Presentation of software operations via the MatCalc GUI. Ther-modynamic equilibrium analysis for typical problems of precipitation reactions

- 10:30 Coffee break
- 11:00 M.Apel

Introduction into the software MICRESS

Setting up a simulation, required material and process parameters, numerical aspects, data analysis and visualisation

12:00 Lunch

Practical demonstrations

13:30 G. Inden

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
- 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 and Dinner, informal get together

Wednesday

Applications: Developments based on Simulations

8:30 G. Inden

Computer-aided materials design

Super heat resistant ferritic steels Complex heat treatments Combined formation and dissolution of particles

9:30 E. Kozeschnik

Precipitation reactions in complex steels

Concurrent precipitation of complex carbides and intermetallic phases in a novel tool steel

- 10:30 Coffee break
- 10:50 B. Böttger

Simulation of microstructure formation during casting, welding and technical heat treatments

Examples of application to various materials as steels, aluminium, magnesium and nickel based alloys

11:50 G. Inden

Closing discussion

Future challenges, outlook on further applications

12:30 End of the seminar

Transformation

Phase

of

Simulation

Registration

4 - 6 July 2011 European Adva Maria-Laach stitute / Com tel, First Nam