

DGM Report to APDIC, May 21, 2011

Deutsche Gesellschaft für Materialkunde, Germany, Austria, Switzerland

Technical Committee:

Thermodynamics, Kinetics and Constitution of Materials

1. Presentations and meetings of the DGM Phase Equilibria and Thermodynamics Committee

(1) The DGM committee "Thermodynamics, Kinetics and Constitution of Materials" and its activities were presented at the annual meeting of the "DGM Technical Committee Organizers" in Darmstadt (Germany), August 23, 2010. All the activities of the DGM committee and APDIC activities were presented. The presentation and actions were positively evaluated and we can expect on-going support by DGM.

(2) A meeting of the technical committee was organized on September 3, 2010 (9am - 3pm) at the Technical University of Freiberg. All participants presented their work and further collaborations are planned. Participants of this meeting were:

- Damian Cupid (TU Freiberg)
- Günter Effenberg (MSI Stuttgart)
- Olga Fabrichnaya (TU Freiberg)
- Michael Fleck (Univ. Bayreuth)
- Peter Franke (TU Freiberg)
- Bronislava Gorr (Univ. Siegen)
- Ulrike Hecht (Access)
- Tim Gestrich (Fraunhofer Inst. IKTS, Dresden)
- Arno Kaiser (RWTH Aachen)
- Andreas Leineweber (MPI Stuttgart)
- Torsten Markus (Research Center Jülich)
- Patrick Masset (TU Freiberg)
- Martin Palm (Max-Planck-Institut Eisenforschung, Düsseldorf)
- Markus Rettenmayr (Univ. Jena)
- Clemens Schmetterer (TU Freiberg)
- Rainer Schmid-Fetzer (TU Clausthal)
- Hans Jürgen Seifert (KIT, Karlsruhe)
- Michael Spiegel (Salzgitter-Mannesmann, Duisburg)
- Frank Stein (Max-Planck-Institut Eisenforschung, Düsseldorf)

(3) A symposium on "Thermodynamics and kinetics: modelling of phase diagrams and microstructure evolution" will be organized at the Euromat 2011 conference (September 12-15, 2011, Montpellier, France).

2. Current phase diagram related activities

Recent work on various systems is detailed in the separate Report Table

3. Seminars

Seminars will be taking place as "European Advanced Training Courses" in Maria

Laach, Germany. These DGM courses have been established as a successful series over the last years. The training courses address materials engineers and scientists in research and development department in industry and at universities.

Simulation of Phase Transformation, July 04-06, 2011
Computer-Aided Thermodynamics, July 06-08, 2011

4. Major research programs involving phase diagram related research with funding in Germany

German Research Foundation (DFG)

Priority Programme SPP 1296:

Heterogeneous nucleation and microstructure formation: steps towards a system and scale-bridging understanding

Duration: 2007 + 6 years (review period 2 years)

Website: <http://www.spp1296.rwth-aachen.de/index.php?id=15>

Alloy systems: Various binary alloys. Also colloidal systems

Contact person for phase diagram and thermodynamics related research: Rainer Schmid-Fetzer.

German Research Foundation (DFG)

Priority Programme SPP 1473:

Materials with new design for improved lithium ion batteries – WeNDeLIB

Duration: 2010 + 6 years (review period 2 years)

Website: to be established

Alloy and ceramic systems: LIB cathode and anode related systems.

Contact person for phase diagram and thermodynamics related research: Hans J. Seifert

German Research Foundation (DFG)

Collaborative Research Center SFB 799:

TRIP-Matrix-Composites, design of tough transformation-strengthened composites and structures based on Fe-ZrO₂

was installed in 2008 at the Freiberg University of Technology.

Duration: 2008 + 12 years (review period 4 years)

Website: <http://tu-freiberg.de/ze/sfb799/index.en.html>

Alloy and ceramic systems: Fe-ZrO₂ based composites; multi component extensions.

Contact person for phase diagram and thermodynamics related research: Hans J. Seifert

German Research Foundation (DFG)

Collaborative Research Center SFB 761:

Steel - ab initio, quantum mechanics guided design of new Fe based materials

was installed in 2007 at Aachen University of Technology (RWTH).

Duration: 2007 + 12 years (review period 4 years)

Website: <http://abinitio.iehk.rwth-aachen.de/index.php?id=1&L=>

Alloy systems: Fe-Mn-C based alloys; multicomponent extensions.

Contact person for phase diagram and thermodynamics related research:
Bengt Hallstedt

German Research Foundation (DFG)

Research Training Group 1229:

Stable and metastable multi-phase systems for elevated service temperatures

was installed in 2006 at Universities of Erlangen and Bayreuth.

Duration: 2006 + 9 years (review period 4.5 years)

Alloy systems: Ni-base superalloys.

Contact person for phase diagram and thermodynamics related research:

Uwe Glatzel

5. Objectives of the DGM Technical Committee

Experimental and theoretical **methods** to determine thermodynamic data and phase diagrams (Ab initio, Phase field, Calphad, ...)

Evaluation of constitutional data and phase diagrams

Thermodynamic **modeling** of multicomponent multiphase materials systems including atomistic approaches

Combination of thermodynamic modelling with simulation of reactor processes as well as with micro- and macrokinetics of microstructure formation in multicomponent and multiphase materials

Development of integrated thermodynamic-kinetic **databases**

6. Goals of the DGM Technical Committee

Use of databases for application oriented computer simulations for **materials- and process optimization**. Cooperation with industrial partners.

Establishing of a **interdisciplinary discussion platform** for fundamental- and application oriented research and development on the working areas.

Organisation of **Sessions** at (international) conferences esp. Europe.

Activities of members should be coordinated in Germany, Austria, Switzerland and integrated into **international activities**:

- (1) Alloy Phase Diagram International Commission, APDIC,
- (2) Scientific Group Thermodata Europe (SGTE),
- (3) ASM International: Phase Diagram Committee,
- (4) TMS: Alloy Phases Committee

Support of instructors in **teaching** of materials thermodynamics, constitution, Kinetics.

Organisation of **DGM training courses**

Initiating of coordinated **proposals** for projects (DFG, BMBF, EU, ...). Joint projects of universities, research institutes and industry.

7. Members of the DGM Technical Committee

| | | |
|---|---|-------------------------|
| Dr. Günter Effenberg | Materials Science Int'l Services GmbH | Stuttgart |
| Dr. Olga Fabrichnaya | TU Bergakademie Freiberg | Freiberg |
| Dr.-Ing. Jörg Fischer-Bühner | | Schwabisch Gmünd |
| Dr. rer. nat. Bernd Gather | Universität Osnabrück | Osnabrück |
| Dr. rer. nat. Bernd Grieb | Magnequench International, Inc. Europe | Tübingen |
| Prof. Dr. Klaus Hack | GTT-Technologies | Herzogenrath |
| Dr. Bengt Hallstedt | RWTH Aachen | Aachen |
| Dr. rer. nat. Mathias Herrmann | Fraunhofer-Institut IKTS | Dresden |
| Prof. Dr. Gerhard Inden | | Ratingen |
| Prof. Dr. Herbert Ipsier | Universität Wien | Wien, Austria |
| Prof. Dr. Hans Flandorfer | Universität Wien | Wien, Austria |
| Dr. Arno Kaiser | RWTH Aachen | Aachen |
| Prof. Dr. Hans R. Kirchmayr | Technische Universität Wien Wien | Austria |
| Dr. Ulrich Klotz | Forschungsinstitut für Edelmetalle & Metallchemie | Schwabisch Gmünd |
| Priv.-Doz. Dr. Guido Kreiner | Max-Planck-Institut für Chemische Physik fester Stoffe | Dresden |
| Prof. Dr. Walter Lengauer | Technische Universität Wien | Wien, Austria |
| Dr. Christian Leinenbach | EMPA | Duebendorf, Switzerland |
| Dr. Hans Leo Lukas | | Waldenbuch |
| Dr. Norbert Mattern | Leibniz-Institut für Festkörper- und Werkstoffforschung | Dresden |
| Dr. Patrick Masset | TU Bergakademie Freiberg | Freiberg |
| Prof. Dr. Eric J. Mittemeijer | MPI für Metallforschung | Stuttgart |
| Prof. Dr. A. Neckel | Universität Wien | Wien, Austria |
| Dr. Martin Palm | Max-Planck-Institut für Eisenforschung GmbH | Düsseldorf |
| Prof. Dr. rer. nat. Dr. h.c. mult. Günter Petzow | Max-Planck-Institut für Metallforschung | Stuttgart |
| Dr. rer. nat. Bernd Reinsch | Robert Bosch GmbH | Stuttgart |
| Dr. Peter Rogl | Universität Wien | Wien, Austria |
| Prof. Dr.-Ing. Rainer Schmid-Fetzer | Technische Universität Clausthal | Clausthal-Zellerfeld |
| Dr. rer. nat. André Schneider | Salzgitter Mannesmann Forschung GmbH | Duisburg |
| Dr. Julius Schuster | Universität Wien | Wien, Austria |
| Prof. Dr. Hans Jürgen Seifert | TU Bergakademie Freiberg | Freiberg |
| Prof. Dr. Ferdinand Sommer | Max-Planck-Institut für Metallforschung | Stuttgart |
| Dr. Frank Stein | Max-Planck-Institut für Eisenforschung GmbH | Düsseldorf |
| Prof. Dr. Josef Tomiska | Universität Wien | Wien, Austria |
| Dr. rer. nat. Henk van den Berg | Kennametal Technologies GmbH | Essen |
| Dr. Peter Waldner | Montanuniversität Leoben | Leoben, Austria |
| Dr. rer. nat. Johannes Weiss | Ing.-Büro Werkstoff-Technik, Qualitäts-Umweltmanagement | Heuweiler |
| Dr. Victor T. Witusiewicz | ACCESS e.V. | Aachen |

Deutsche Gesellschaft für Materialkunde, Germany, Austria

Upcoming Report Table, to be published after the next APDIC meeting

This table is accessible for contributors to Deutsche Gesellschaft für Materialkunde, Germany, Austria only.

This table accumulates entries until the next APDIC meeting.

After the meeting, the table will be edited by the representatives of Deutsche Gesellschaft für Materialkunde, Germany, Austria, and transferred on their initiative to the public area of the APDIC Web.

Just after the next APDIC meeting, a new empty table will start to collect entries for the next annual report.

EP: Experimental Work on Phase Equilibria

ET: Experimental Work on Thermodynamic Data

CA: Experimental Work on Properties or Applications

CT: Computational Thermodynamic Calculations (Calphad)

CA: Computational Atomistic Calculations
 ICE: Intellectual Critical Evaluation of All Published Data

Materials System EP ET CA CT ICE Comment Contributor

| | | | | | | | | | |
|----|--------------------------------|---|---|---|---|---|------------------------------|----------------------------|--------------------------|
| 1 | Al | | | | F | F | | PhysChemMin 37,2010,721 | Rainer Schmid-Fetzer |
| 2 | Al-B-C-Nb-Ti | P | P | | P | | | | Dr. Victor T. Vitusevych |
| 3 | Al-Bi-Si | F | F | | F | F | J.Mat.Sci 45, 2030(2010) | | Rainer Schmid-Fetzer |
| 4 | Al-C-Ce-O-Si-Y | F | | | | | IJMR 101 (11) (2010) 1405 | | Hans Juergen Seifert |
| 5 | Al-C-N-O-Si-Y | | | | X | | | | Hans Juergen Seifert |
| 6 | Al-C-O-Si-Y | | | | F | F | JPED 31 (2010) 238-249 | | Hans Juergen Seifert |
| 7 | Al-C-Ti | | | | X | | | | Bengt Hallstedt |
| 8 | Al-C-V | | | | X | | | | Bengt Hallstedt |
| 9 | Al-Ca-Fe-O-Si | X | X | X | P | X | | | Patrick J. Masset |
| 10 | Al-Cu | | | | P | | | | Bengt Hallstedt |
| 11 | Al-Cu-Mg-Si | | | | X | X | | | Rainer Schmid-Fetzer |
| 12 | Al-Cu-Si | X | X | | X | X | | | Rainer Schmid-Fetzer |
| 13 | Al-Cu-Si | | | | P | | | | Bengt Hallstedt |
| 14 | Al-Fe | F | | | | | | | Frank Stein |
| 15 | Al-Fe-Mn | | | | X | | | | Bengt Hallstedt |
| 16 | Al-Gd-O-Y-Zr | F | | | F | | J. Phase Equilibria and D | | Hans Juergen Seifert |
| 17 | Al-Ge-Sn | X | | | | | emf measurements | | Herbert Ipser |
| 18 | Al-Mg-Si | X | X | | X | X | | | Rainer Schmid-Fetzer |
| 19 | Al-Mg-Si | | | | X | | | | Bengt Hallstedt |
| 20 | Al-Mo-Ti | | | | F | F | Intermetallics 18 (2010) | | Hans Juergen Seifert |
| 21 | Al-Ni | F | F | | F | F | ThermochimActa 512,2011,1 | | Rainer Schmid-Fetzer |
| 22 | Al-O-Y-Yb-Zr | X | | | X | | | | Hans Juergen Seifert |
| 23 | Al-O-Yb-Zr | F | | | F | | Calphad 34 (2010) 206-214 | | Hans Juergen Seifert |

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|----|---|-------|-------------------------------|--------------------------|
| 24 | Al-Ta-Ti | F F F | | Dr. Victor T. Vitusevych |
| 25 | Bi-Cu-Sn | F F | F F to be published | Rainer Schmid-Fetzer |
| 26 | C-Cr-Cu-Fe-Mg-Mn-Mo-Ni-Si | | F AEM 12, 158(2010) | Bengt Hallstedt |
| 27 | C-Fe | F F | Calphad 34, 129(2010) | Bengt Hallstedt |
| 28 | C-Fe-Mn | | X | Bengt Hallstedt |
| 29 | C-Fe-Mn | | F Calphad, submitted, 2011 | Bengt Hallstedt |
| 30 | C-Fe-N | X X | IJMR 98, 1086 (2007) | Eric J. Mittemeijer |
| 31 | C-Li | | X X | Rainer Schmid-Fetzer |
| 32 | C-Mn | F F | Calphad, under review | Bengt Hallstedt |
| 33 | C-Mn | | F Calphad, 34, 279-85(2010) | Bengt Hallstedt |
| 34 | Ca-Ce-Mg-Sn | F F | F F to be published | Rainer Schmid-Fetzer |
| 35 | Ca-Mg-Si-Sn | F F | F F JALCOM 509 2011, 3326 | Rainer Schmid-Fetzer |
| 36 | Cd-Ce | | X vapor pressure measurement. | Herbert Ipser |
| 37 | Cd-Ce | X X | | Herbert Ipser |
| 38 | Cd-Gd | | X vapor pressure measurement. | Herbert Ipser |
| 39 | Cd-Gd | X X | | Herbert Ipser |
| 40 | Cd-Nd | P P | | Herbert Ipser |
| 41 | Ce-Gd-Mg-Y | | F F Scripta Mater. 63, 2010, | Rainer Schmid-Fetzer |
| 42 | Ce-La-Mg | F F | F F to be published | Rainer Schmid-Fetzer |
| 43 | Ce-Mg-Nd | F F | F F Acta Mater., 59 2011, 613 | Rainer Schmid-Fetzer |
| 44 | Ce-Mg-Zn | F F | F F Intermet.18 (2010) 399 | Rainer Schmid-Fetzer |
| 45 | Cr-Fe-Mn-Ni | X | X | Hans Juergen Seifert |
| 46 | Cr-Fe-Ni | | F CALPHAD 35 (1) (2011) 148 | Hans Juergen Seifert |
| 47 | Cu-Ni-Sn | F | | Herbert Ipser |
| 48 | Cu-Si | | P | Bengt Hallstedt |
| 49 | Cu-Si | | X X | Rainer Schmid-Fetzer |

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|----|---------------------------|---------|-------------------------------|--------------------------|
| 50 | Fe | F F F | PhysChemMin 37,2010,721 | Rainer Schmid- Fetzer |
| 51 | Fe-H-Mn | X | | Bengt Hallstedt |
| 52 | Fe-H-Mn | F | Steel Res Int 82, 108-13 | Bengt Hallstedt |
| 53 | Fe-Mn-Nb | X | | Bengt Hallstedt |
| 54 | Fe-Nb | X | | Frank Stein |
| 55 | Fe-Nb | X | | Bengt Hallstedt |
| 56 | Fe-Ni-Si | F | AEM 12, 158(2010) | Bengt Hallstedt |
| 57 | Ga-Ni | F | | Herbert Ipser |
| 58 | Gd-Mg | F F | | Rainer Schmid- Fetzer |
| 59 | Gd-Mg-Zn | X X X X | | Rainer Schmid- Fetzer |
| 60 | In-Sn | F | | Herbert Ipser |
| 61 | In-Sn-Zn | F | | Herbert Ipser |
| 62 | La-Mg-Nd | X X X X | | Rainer Schmid- Fetzer |
| 63 | La-O-Y-Zr | F F | J. Alloys and Compounds 5 | Hans Juergen Seifert |
| 64 | Li-Ni-O | P | | Bengt Hallstedt |
| 65 | Li-O | F | Calphad, 35, 160- 64(2011) | Bengt Hallst |
| 66 | Mg-Nd | F F | | Rainer Schmid- Fetzer |
| 67 | Mg-Si | X | | Bengt Hallstedt |
| 68 | Mg-Si-Sn | F F F F | JALCOM 509 2011, 3326 | Rainer Schmid- Fetzer |
| 69 | Mg-Y-Zn | X X X X | | Rainer Schmid- Fetzer |
| 70 | N-Nb | F | Calphad 33, 233(2009) | Bengt Hallstedt |
| 71 | Nd-O-Y-Zr | F F F F | IJMR 101 (11) (2010) 1354 | Hans Juergen Seifert |
| 72 | Ni-P | F F | | Herbert Ipser |
| 73 | Ni-P | F | | Herbert Ipser |
| 74 | Ni-P-Sn | F | | Herbert Ipser |
| 75 | Ni-Sb-Sn | X X P | | Herbert Ipser |
| 76 | Ni-Sb-Sn | F F | | Herbert Ipser |
| 77 | P-Sn | X F | | Herbert Ipser |
| 78 | P-Sn | F | | Herbert Ipser |