Report to APDIC for year 2022
Deutsche Gesellschaft für Materialkunde e.V. (DGM, German Materials Society), Germany, Austria, Switzerland

Technical Committee: Thermodynamics, Kinetics and Constitution of Materials (Contact person: Hans Jürgen Seifert, Karlsruhe Institute of Technology, KIT IAM-AWP)

1. **General activities of the DGM Thermodynamics, Kinetics and Constitution of Materials Committee. Organizers and Co-Organizers of Conferences.**

(1) **45th *International Conference & Exhibition on Advanced Ceramics & Composites, ICACC 2022*** (Jan 23 - 28, 2022), the symposium S10: "**Modeling and Design of Ceramics and Composites**" was co-organized by Hans Seifert, KIT (Main organizer: Jingyang Wang, Inst. of Metal Research, Chinese Academy of Sciences; International committee with 12 organizers in total).

(2) ***35th Annual MSIT Meeting - International Seminar on the Evaluation of Heterogeneous Multicomponent Equilibria***" (03-08 April 2022, Online only event). The annual one-week seminars are organized by the Materials Science International Team, MSIT, Stuttgart. Organizing team: Svitlana Iljenko (MSI, Materials Science International GmbH, Germany), Andrew Watson (Hampton Thermodynamics, Ltd., UK), Frank Stein, Martin Palm (both Max-Planck-Institut für Eisenforschung GmbH, Germany). About 50 experts from academic institutions worldwide participated. Aim: Literature data evaluation for ternary systems and writing system reports. In parallel the **6th MSIT Winter School on Materials Chemistry** was organized.

(3) **Materials Science and Engineering, MSE Congress (online)**
(27-29 September 2022, Darmstadt, Germany)
Topic Modeling and Simulation, Symposium M05 "Computational and Experimental Thermodynamics and Kinetics of Materials"
Organized by: H.J. Seifert (KIT), Y. Du (CSU, Changsha, China), E. Gamsjäger (Montanuniversität Leoben, Austria), T. Markus (Hochschule Mannheim), R. Schmid-Fetzer (TU Clausthal)
(about 20 oral and poster presentations)
This symposium focuses on fundamental aspects of the thermodynamics of materials and the kinetics of microstructure evolution associated with non-equilibrium states, phase transformations and defects. Experimental and computational approaches comprise but are not limited to: CALPHAD-type modeling, First-principle and Monte-Carlo methods, Phase Field approaches, experimental phase diagram investigations (materials constitution), experimental thermodynamics and kinetics. Materials of interest are metals and ceramics, respectively. However, applications referring to composites, soft matter and biological materials are welcome to explore synergetic approaches.

Also theory and applications of thermodynamics and kinetics for “materials behavior in engineering systems”, e.g. for energy storage and conversion, are welcome.

(4) **18th Discussion Meeting on Thermodynamics of Alloys**, Krakow, Sep 12-16, 2022
International Advisory Committee, members from Germany: J. Brillo, O. Fabrichnaya, S.G. Fries, H.J. Seifert, F. Stein

(5) **GTT Users´ Meeting** (online), June 29-24, 2022, Herzogenrath
About 150 participants

2. Major (coordinated) research programs involving phase diagram related research with funding in Germany

German Research Foundation (DFG)
Priority Programme (SPP2006), „Compositional Complex Alloys – High Entropy Alloys (CCA-HEA)
Is funded since year 2017
Duration: 2017 + 6 years
Website: https://www.sppccahea.uni-bayreuth.de/en/index.html

German Research Foundation (DFG)
Research Group (FOR 3010) REFRABUND
Is funded since year 2020 (Technical University of Freiberg and KIT; total of seven projects)
Duration: 2020 + 6 years
Refractory composites from Niobium-Alumina and Tantalum-Alumina, respectively

German Research Foundation (DFG)
Research Training Group, Graduate School 2561 “Materials Compounds from Composite Materials for Applications in Extreme Conditions”
Is funded since year 2020 (Technical University of Darmstadt and KIT)
Duration: 2020 + 6 years
Total of 13 projects on engineering materials in the system Mo-Ti-Si-B-X

German Research Foundation (DFG)
Collaborative Research Center, SFB/CRC 1394 “Structural and Chemical Atomic Complexity – From Defect Phase Diagrams to Materials Properties”
Is funded since year 2020 (RWTH Aachen) and is planned for 12 years duration. All 18 projects work on materials system Mg-Al-Ca, its solid solutions, intermetallic phases and the creep-resistant in-situ composites of both.

German Research Foundation (DFG) and National Natural Science Foundation of China (NSFC); The Sino-German Center for Research Promotion in Beijing (SGC)
Sino-German Cooperation Group “Integrated Computational Materials Engineering of Electrochemical Storage Systems”
Duration: 36 months since 2019 (extended to 06/2024 due to pandemic situation)
Collaboration Partners: Central South University, Changsha (Yong Du), Guilin

University (Li-Xian Sun), KIT (Hans Seifert)
In this project, modeling and simulation tools of ICME (Integrated Computational Materials Engineering) supported by key experiments and electrochemical cell testing will be used for rational and efficient design of new high performance lithium batteries. For cell design, we will combine new type of high voltage cubic spinel cathode materials with intermetallic tin-base anode alloys, embedded in Ga-rich liquid matrix, showing strong volume buffer and self-healing effects, respectively.

3. 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***

4. Specific 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 plattform** 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,
(5) The American Ceramic Society: Phase Equilibria 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.

5. Members of the DGM Technical Committee

Böttger, Berndt (Access, Aachen)
Fabrichnaya, Olga (TU Bergakademie Freiberg)
Flandorfer, Hans (Univ. Wien)
Gorr, B. (Univ. Siegen)
Hack, Klaus (GTT Technologies, Herzogenrath)

Hallstedt, Bengt (RWTH Aachen)
Herrmann, Mathias (Fraunhofer-Institut IKTS, Dresden)
Iljenko, Svitlana (MSI, Stuttgart)
Kaiser, Arno (Fraunhofer-Institut IKTS, Dresden)
Klotz, Ulrich (Forschungsinstitut für Edelmetalle und Metallchemie, Schwäbisch-Gmünd)
Leinenbach, Christian (EMPA)
Leineweber, Andreas (TU Bergakademie Freiberg)
Lippmann, Stephanie (Univ. Jena)
Markus, Torsten (Hochschule Mannheim)
Palm, Martin (MPI Eisenforschung)
Schneider, André (Vallurec, Düsseldorf)
Schmid-Fetzer, Rainer (TU Clausthal)
Schmitt, Lisa-Yvonn (Forschungsinstitut für Edelmetalle und Metallchemie, Schwäbisch-Gmünd)
Seifert, Hans Jürgen (Karlsruhe Institute of Technology, KIT)
Spatschek, Robert (Research Center Jülich)
Stein, Frank (MPI Eisenforschung, Düsseldorf)
To Baben, Moritz (GTT Technologies, Herzogenrath)