



**Report to APDIC for year 2023**  
**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) **34<sup>th</sup> Annual MSIT Meeting - International Seminar on the Evaluation of Heterogeneous Multicomponent Equilibria** (12-16 March 2023). 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). **7<sup>th</sup> MSIT Winter School on Materials Chemistry** was organized.
- (2) **25<sup>th</sup> GTT Users' Meeting** (online), June 20-21, 2023, Herzogenrath  
About 150 participants (Organizer: M. To Baben and team)
- (3) **25<sup>th</sup> Thermo-Calc User Group Meeting** (online), March 30-31, 2023, Aachen  
(Organizer: N. Grundy and team)

**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) REFRA-BUND**

Is funded since year 2020

TU Freiberg and Karlsruhe Institute of Technology (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 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,

(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)