

# Materials Research Department

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**RU**B

### Welcome to the 2021 MRD Newsletter!

#### DEAR READERS,

some of you will remember that our last issue was published in German. Its focus was on reaching out to colleagues from companies and research laboratories in our region and to report on applied materials research activities at our university. This year we return to English and focus on collaborative materials related research programs at our university. We first present a short description of our Materials Research Department. We then present a few collaborative research centers and show some results which were produced from projects embedded in these activities. Our university takes part in two International Max Planck Research Schools and we provide details on the development of these schools and plans for the future. There have been changes in the management of our MRD. In April 2021, Felicitas Scholz has taken over as one of our two science managers from Axel Marquardt, who has taken up a position in industry. Together with Pia Aleithe, she is responsible for the day to day running of our MRD. We thank Axel Marguardt for his efforts and welcome Felicitas Scholz on board. We are happy to report that we were able to strengthen the role of the young materials researchers (YMRs) in our MRD this year. We warmly welcome Isabel Pietka and Kevinjeojios Pellumbi as new members of our MRD board, who were elected by the YMR community in June 2021.

The present MRD board (C. Bock, A. Devi, R. Drautz, G. Eggeler, A. Grünebohm, R. Janisch, J. Pfetzing-Micklich, J. Schreuer, A. Wieck and the two newly elected representatives of the YMRs) has been elected for the period 2020/21. According to our MRD procedures, a new board will be elected for the years 2022 and 2023. The election will take place in our members meeting on December 6th, 2021. Information will be provided in due course. We are always looking forward to receiving feedback on our newsletter and on all of our activities. Please send your suggestions and questions to mrd@rub.de.

Enjoy reading,

P. Aleithe, R. Drautz, G. Eggeler and F. Scholz



MRD speakers Ralf Drautz (left) and Gunther Eggeler (right) and science managers Pia Aleithe (middle left) and Felicitas Scholz (middle right).

### Research at RUB's Materials Research Department (MRD)

The hierarchical nature of materials necessitates interdisciplinary materials science: Materials are ubiquitous. They affect every aspect of our daily lives. They are the basis for today's cutting edge technologies and the availability of novel materials and efficient processing routes determine the pace at which innovations can proceed. This makes materials important to help mankind to find the right technological answers in the fields of energy, transport, health, housing and environment. Materials science is an interdisciplinary research field. Its traditional focus on structure-property relationships of structural engineering materials has long been broadened. Today's materials science comprises materials chemistry and physics, mechanics and thermodynamics of materials. Combinatorial materials research and materials informatics are new fields, which provide valuable new contributions. Materials for medical applications and biological materials and new technologies, like coating procedures and additive manufac-









Scale bridging journey from the nanocosmos into the macro scale of a superalloy turbine blade.



Movie - From atoms to turbine blades

turing, are receiving attention. Therefore, materials researchers often belong to different academic departments and have diverse backgrounds. In RUB's Materials Research Department (MRD), materials researchers from all disciplines with their specific areas of expertise join forces to progress the field.

In the past it was quite common that phenomena, which are associated with specific length scales (electronic, atomic, microstructural and macroscopic), were studied separately. Today there is a strong emphasis on understanding scale-bridging aspects of materials science. To this end the hierarchical structure of materials needs to be explored: Electrons form chemical bonds between atoms. Depending on bond chemistry, temperature and pressure the atoms arrange themselves in different ways. For example, atoms form gases and liquids and in the solid state crystals or glasses. The defects of crystalline solids and the arrangement of atoms in an amorphous material have a strong influence on macroscopic material properties. For example, atomic diffusion processes limit the exploitable service life of a superalloy turbine blade. The strength of chemical bonds determines the energy density of batteries. The ability to process materials with atomic scale precision is decisive for electronic transport in semiconductor devices. Thus, materials research is rooted in the hierarchical structure of materials, which promotes the interdisciplinary character of the field.

Today, for each hierarchical level/length scale, characterization, processing and simulation methods are available. A key challenge for materials science consists in the design and development of novel materials with desired properties, and the improvement of conventional materials in terms of performance, exploitable service lives and sustainability. This requires bringing together expertise from various fields and well-defined, targeted interdisciplinary research efforts. It further requires the identification of limitations and shortcomings of available methods and, most importantly, establishing bridges between length scales. To this end in particular, data and information from each materials hierarchy need to be aggregated and analyzed. The MRD provides an ideal frame to stimulate this type of interaction. It also aims at acting as a platform for collaborative research efforts, where interdisciplinary expertise is required.

Strategy of the Materials Research Department: Over the past years the MRD has implemented a structure that enables the seamless study of materials across length scales. The Institute of Materials (IM) at RUB acted as a nucleus that was instrumental for establishing the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and the RUB Research

Centre ZGH (Centre for interface dominated high performance materials). Together the IM, ICAMS and ZGH provide the core expertise and facilities for the MRD that enable the characterization, processing and simulation of materials across all materials hierarchies, a unique characteristic of RUB's MRD. This core expertise is currently being extended to include data science and materials informatics for a seamless integration of data and information form the different materials hierarchies. The MRD core formed by IM, ICAMS and ZGH provides ample opportunities for research in close collaboration with MRD members that have their main affiliation in other departments and disciplines. Here, MRD promotes the interaction of researchers from different fields and helps to initiate collaborative research. In fact, materials design has become a relevant research topic in other departments of RUB, for example in chemistry, geo-sciences, mathematics, medicine and physics.

Diversity is a necessity for vivid exchanges and excellent research collaborations within the MRD. The promotion of early career researchers and their active contributions to MRD research are another key element of the MRD strategy. The MRD seeks to further strengthen materials science expertise at RUB by attracting new faculty members and by further strengthening interdisciplinary interactions not only between all RUB reserarchers with interest in materials research but also with all associated academic colleagues from research institutions close to RUB, like the Max-Planck-Institutes for Iron Research, Coal Research and for Chemical Energy Conversion (MPIE, MPIK and MPICEC), the German Centre for Aerospace Research (DLR) and the Research Centre Jülich (FZ Jülich). It also promotes scientific and technological exchange with research colleagues from R&D departments of the materials industry surrounding RUB. The MRD is coordinating the activities of RUB in the UA Ruhr flagship program Materials Chain, a collaborative research framework of Ruhr-Universität Bochum, the University of Duisburg-Essen and TU Dortmund University. All members of the MRD are also members of the Materials Chain.

In summary MRD's research strategy focusses on (i) establishing research expertise and facilities for materials science across length scales, (ii) fostering interdisciplinary scientific interactions at RUB integrating nearby institutions and international partners, (iii) promoting early career researchers and (iv) interacting with industrial R&D departments from the Ruhr Area. This forms the basis for our current efforts to coordinate RUB's next proposal for an excellence cluster in materials science. In this way, MRD con-



Website of the MRD

#### FIGURE 2

Multiscale modelling of materials across the length scales (After D.G. Pettifor, 1991). For more information see here:





Website of ICAMS

Fruitful discussions on a poster session at the Young Materials Researcher Day in 2018.



tributes to strengthening both, RUB's visibility in the international scientific materials community as well as RUB's integration in the technological material developments in our Ruhr Area.

Main research topics: The MRD is a stronghold for research in structural and functional engineering materials, like superalloys, shape memory alloys and advanced steels. New catalytic materials, semiconductors, superconductors and magnetic materials are also important and represent exciting research topics. In recent years, materials issues related to hydrogen technology and sustainable materials technologies have received increased attention. Contributions are made to develop processing routes from atomic layer deposition to bulk samples, including combinatorial high-throughput methods, additive manufacturing and plasma-based methods. These are accompanied by method developments for characterizing and simulating materials across all length scales. Members of the MRD lead a number of large collaborative research projects.

**Organization of MRD research:** The members of the MRD elect for the duration of two years the speaker of the MRD, the deputy speaker and the MRD board that represents RUB's materials research. Two science managers assist the speakers in the organization of the MRD and its contributions to the Materials Chain. The members of the MRD are selected based on merit and elected by the MRD general assembly. Among the regular meetings that the MRD organizes are the general assembly, Materials Day, Young Materials Researchers Day, Industry Day as well as workshops and conferences, for example, together with the Materials Chain research framework.



### SFB/TR 103 – From atoms to turbine blades - a scientific basis for a new generation of single crystal superalloys

The SFB/Transregio 103 is a collaborative research center funded by the German Research Association DFG. It has reached its third four year finding period and focusses on Ni-base superalloy single crystals (SX). SX represent key materials for turbine blades in modern gas turbines for aero engines and power plants. International mobility and global energy supply rely on SX. Improvements in efficiency and emissions demand new concepts in the areas of (i) basic understanding of all aspects of alloy design and performance, (ii) continuous improvement and innovation of processing technologies, (iii) scale bridging characterization of nano-/microstructures and properties, (iv) scale bridging materials modelling and (v) efficient handling of research data. The research activities of SFB/TR 103 focus on two central questions: What is the role of large and small-scale microstructural heterogeneities (large-scale heterogeneity: dendrites and interdendritic regions, small-scale heterogeneity:  $\gamma/\gamma$ '-microstructure)? How do alloy elements (especially: d-shell elements like Re, W, ...) affect microstructure, microstructural evolution and properties? From a fundamental point of view it is important to understand how these parameters affect thermodynamic equilibria, the evolution of microstructure during processing and high temperature exposure and high temperature strength. Modern alloy design strives for better performance in terms of most efficient use of fossil resources. It must also respect the limited availability of strategic elements (e.g. less Re, more W, Mo and others). In addition to Ni-base

G. Eggeler



Website of SFB/TR to:

Mechanical properties					
A1	B1	C1	T2(C6)		
A2	B2	C2	T3(C4)		
<b>A</b> 3	B3	C3	T4(B4)		
A4			T5(B6)		
A5	B5	C5			
A6					
A7	B7	C7			
	B8				

Co-ordinator: M. Bartsch



Co-ordinator: C. Körner



SFB/Transregio 103 SUPERALLOY SINGLE CRYSTALS 

#### Motorials information

materials informatics					
A1	B1	C1	T2(C6)		
A2	B2	C2	T3(C4)		
A3	B3	C3	T4(B4)		
A4			T5(B6)		
A5	B5	C5			
A6	B6				
A7	B7	C7			
	B8				

Co-ordinator: T. Hammerschmidt

Alloy development					
A1	B1	C1	T2(C6)		
A2	B2	C2	T3(C4)		
A3	B3	C3	T4(B4)		
A4			T5(B6)		
A5	B5	C5			
A6					
A7	B7	C7			
	B8				

Co-ordinator: S. Neumeier

Thermodynamics and kinetics

A1	B1	C1	T2(C6)	
A2	B2	C2	T3(C4)	
A3	B3	C3	T4(B4)	
A4			T5(B6)	
A5	B5	C5		
A6	B6			
A7	B7	C7		
	B8			
Co-ordinator: R Drautz				

-ordinator: R. Draut

FIGURE 1 22 projects of

SFB/TR 103 and their participation in cross sectional groups.

superalloys, an effort is made to explore the high temperature properties of new Co-based single crystal superalloys with  $\gamma/\gamma'$ -microstructures.

In SFB/Transregio 103, the Ruhr-Universität Bochum (RUB) and the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) join forces and collaborate with the MPIE, Düsseldorf, the DLR, Köln and the FZ Jülich. Different areas of expertise, including materials science and engineering, solid state physics and chemistry, scale bridging materials modeling and processing and manufacturing technology are in close scientific contact. Research in the second third funding period of SFB/TR 103 will tackle open questions related to processing of superalloy single crystals, to the stability of microstructures at high temperatures and to elementary deformation and damage mechanisms. A total of 22 scientific projects participates in SFB/TR 103, which are part of topical blocks but also participate in six scientific cross sectional groups (Figure 1). The Ruhr-University leads this activity and 11 projects from RUB participate in the program. In the present MRD newsletter, some of the SFB/TR 103 projects will briefly describe their projects and present a few research highlights.

F. Scholz, P. Thome, J. Frenzel

# Fundamental aspects of single crystal solidification processing

Project B7 of SFB/TR 103 aims at contributing to a better understanding of the formation and nature of crystal defects in single crystal Ni-base superalloys. In addition, in this funding phase, the need for applying and validating data science approaches for the analysis and interpretation of microstructures and thermomechanical properties represents a new challenge. We use a Bridgman seed technique for single crystal solidification experiments, which allows to precisely control all parameters, which govern solidification [I]. Figure I shows the Bridgman furnace which is used in project B7.

A special effort is made to investigate the formation and evolution of crystal mosaicity in sin-



#### FIGURE 1

Bridgman furnace at the Institute for Materials.

gle crystal Ni-base superalloys. In general, mosaicity is a measure of the spread of crystal plane orientations. A superalloy single crystal exhibiting mosaicity is typically characterized by the presence of small sub grains with misorientations of up to a few degrees. We show that crystal mosaicity is associated with dendrite deformation processes [2]. Therefore, we develop a new tomographic method, which is based on serial sectioning. In a first step, optical micrographs of as-cast superalloys are obtained by a quantitative metallographic procedure using precisely aligned montages of large numbers of optical micrographs. In a second step, neuronal network-based techniques are applied to detect and to evaluate the growth behavior of a large number of individual dendrites, to determine their growth trajectories and to investigate local dendrite spacings.

This approach allows to study the evolution of microstructures by monitoring the growth behavior of more than 2500 dendrites. Sudden changes in growth directions can be observed and documented. These types of orientation defects are related to dendrite bending which is based on a slight rotation of the crystal lattice due to local stress fields. Furthermore, using tomographic microstructure snapshots, we can document how dendrite branching and the interaction between slightly misaligned individual dendrites affect the microstructural features after solidification. Figure 2 illustrates critical steps of our new tomographic analysis method.

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Website of project B7 of SFB/TR 103



#### FIGURE 2

Evaluation of tomographic microstructural information. The growth directions of dendrites are analyzed in terms of polar and azimuth angles. Two isolated dendrites marked by blue arrows are characterized by growth trajectories, which slightly deviate from the main solidification direction.

I. Pietka, M. Forti, T. Hammerschmidt, R. Drautz

### Atomistic modelling of extended defects and machine learning approach for TCP phases in Ni- and Co-base superalloys

Project CI of SFB/TR 103 relates local atomic geometry at defects and interfaces to local bond chemistry in single-crystal Ni-base and Co-base superalloys. In particular, we investigate the influence of alloying elements on phase stability, dislocations, planar faults and internal interfaces. Structure maps and atomistic simulations with density functional theory, tight-binding and bond-order potentials are employed to derive  $\gamma/\gamma'$  alloying windows and to analyze the influence of alloying elements on deformation mechanisms [1,2]. The project has two main efforts. In her Ph.D. project Isabel Pietka develops and applies bondorder potentials for multi-component Ni-based superalloys for simulating segregation to dislocations, planar defects and interfaces. The segregation affects defect properties and the aim of the analysis is to unravel the relation between segregation and formation energy and mobility of the defects. To this end high-throughput calculations with density functional theory are carried out as well as large atomistic simulations with bond-order potentials.

#### FIGURE 1

Binding energy of Re at an edge dislocation as predicted by analytic bond-order potentials.





Three-dimensional structure map. The map enables the prediction of homogeneous phase stability from a few parameters only.

Mariano Forti's postdoc project has its focus on data analysis and aggregation. To this end Mariano employs machine learning in combination with physically motivated descriptors to analyze and predict phase stability of complex topologically close-packed phases. He furthermore develops models for optimizing alloy compositions and predicting ordered  $\gamma'$  phase compositions. Mariano Forti also brings together data generated in the consortium with the aim of providing FAIR datasets in coordination with the national research data initiatives FAIRmat and NFDI-MatWerk.

#### References

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Website of project CI of SFB/TR 103

M. Rajkowski, M. Schneider, G. Laplanche



Website of project B8 of SFB/TR 103

### High entropy alloys

Single-crystal superalloys are two-phase materials consisting of y'-cubes, with an ordered L12 crystallographic structure, that are embedded in a disordered face-centered cubic (FCC) y-matrix. From a fundamental viewpoint, it is of prime importance to characterize the intrinsic properties of these two phases to provide a better understanding of superalloys and guide alloy design. In this context, project B8 of SFB/TR 103 focuses on single-phase FCC alloys, whose compositions correspond to those of the y-matrices in superalloys. Such alloys are chemically complex and their chemical complexity is reminiscent of the high and medium entropy alloys (HEAs and MEAs), which have been investigated with the highest intensity during the last decade. For instance, the y matrix of Ni and Co-based superalloys contains high concentrations of Ni, Co, and Cr and is therefore chemically similar to the ternary CrCoNi MEA, which exhibits outstanding mechanical properties [1,2]. Each of the constitu-

In the following, a few ongoing activities are presented. The y-matrix of a Co-based superalloy developed at the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) was selected and its composition was simplified to obtain a quaternary (Cr, Co, Ni, W) alloy. From this reference γ-matrix, four additional alloys were designed in which the concentration of one of the four elements was reduced by 5 at. % and balanced by increasing the concentrations of the three other elements and keeping the atomic ratios between them constant. These alloys were vacuum induction melted, homogenized and rotary swaged to produce rods. The cold-worked alloys were subsequently annealed for 1000 h in evacuated silica tubes to investigate their stability. In particular, it was found that all the alloys become single-phase FCC above 800 °C, see Figure 1. Based on this knowledge, diffusion experiments are planned to determine how diffusion kinetics is affected by different chemical environments. For this pur-



#### FIGURE 1

Phase stability of the reference  $\gamma$  matrix and four additional alloys after 1000-h anneals at 800 and 900 °C. The backscatter electron images show that all the alloys become single-phase FCC above 800 °C.

ting elements affects a variety of properties and it is, therefore, a challenge to predict how alloy properties will be influenced by changes in chemical composition. In order to enable further optimization of superalloys, there must be systematic investigations into the influence of individual alloying elements on several aspects. Project B8 serves this purpose by investigating the influence of Co, Ni, Cr, and W, on phase stability, diffusion kinetics, the energy of planar defects, all of which are playing major roles in creep of superalloys. pose, the four modified quaternary alloys were assembled in diffusion multiples containing six distinct pseudo-binary diffusion couples (Figure 2), and these will be encapsulated into vacuumed silica tubes and annealed for 100 h between 900 °C and 1200 °C. The resulting chemical diffusion profiles will be investigated by electron dispersive X-ray spectroscopy and compared with different modelling approaches.



Diffusion multiple used in interdiffusion experiments (Master thesis of Maik Rajkowski). (Left) Six pieces corresponding to four distinct alloys. (Middle) Stainless-steel clamping device. (Right) Pieces assembled into a diffusion multiple.

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### Uncovering process-structure relationships through novel microstructural characterization and data analysis

Predicting the effect that chemistry and processing have on the microstructure of any material is a highly valuable proficiency. The morphological and micromechanical properties of individual phases and features, together with the nature of their interactions, are ultimately responsible for the emerging mechanical properties. Deep knowledge of this cause-effect chain is critical to enabling the tailored materials design, the core topical subject of the ever-digitizing fields of Materials Science and Technology.

There are countless ways to characterize the links that form that chain. Arguably, the most widespread technique for microstructural analysis in research and development is scanning electron microscopy (SEM). Its popularity, however, does not mean that its descriptive potential has been exhausted. On the contrary, we believe that it is highly profitable to complement this already incredibly fruitful imaging technique. The motivation within our group to model and describe the manufacturing process and microstructure of powder metallurgy ledeburitic tool steels was the driving force behind the development of general tools that could find application in various materials and systems.

We have developed a novel image analysis strategy to comprehensively characterize closed shapes and their spatial distribution [I] and an algorithm to recover three-dimensional powder distributions from two-dimensional sections [2]. By combining these approaches, we uncovered new process-structure links associated with the hot isostatic pressing of a commercially available high-speed steel [3]. Figure I shows a flowchart of the study published in our last work. We described for the first time how the solidification during atomization influences the final microstructure.

These findings hinge on the fact that SEM images contain an untapped wealth of two and three-dimensional data. We are exploring ways to improve how we analyze our information through convolutional neural networks, an already established tool to extract knowledge from images. In doing so, we intend to produce high-



S. Benito.

S. Weber

Open access to paper in Materials & Design

Flowchart of the synergistic combination of phase analysis and stereology.



throughput schemes to describe systematically different alloy systems and powder atomization parameters.

Finally, we are actively searching for new areas of expertise to deploy our methods and findings. As we devised our algorithms on the premise of versatility, we can employ them in the analysis of closed shapes and particulate systems in a general sense. Some examples include crack and fracture mechanics, meteoritics, or planetary sciences.

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## CRC/TRR 247 "Heterogeneous oxidation catalysis in the liquid phase – mechanisms and materials in thermal, electro-, and photocatalysis"

The CRC/TRR 247 "Heterogeneous Oxidation Catalysis in the Liquid Phase – Mechanisms and Materials in Thermal, Electro-, and Photocatalysis" aims at bringing heterogeneous oxidation catalysis in the liquid phase to a level of fundamental understanding that is comparable to metal catalysis in the gas phase, i.e. to unravel the nature of the catalytically active sites and the reaction mechanisms. It started in 2018 and is currently applying for its second funding period. The first funding period is devoted to the establishment of experimental structure-activity correlations and theoretical modelling of the active site candidates. In the second funding period, we will converge theory and experiment and address the reaction mechanisms. Additionally, we will start to generalize the results to other oxide catalysts. The CRC/TRR 247 includes 21 projects, which are divided into four categories.

The investigated catalysts are cobalt oxides promoted with other metal ions such as iron, which are applied as nanoparticles (NPs) in suspensions or deposited on electrodes. The focus is on spinels (Co<sub>3</sub>O<sub>4</sub>, CoFe<sub>2</sub>O<sub>4</sub>) and perovskites (LaCoO<sub>3</sub>, LaFeO<sub>3</sub>), which allow systematic substitution studies (Co<sub>3-x</sub>Fe<sub>x</sub>O<sub>4</sub>, La<sub>1-x</sub>Sr<sub>x</sub>Co<sub>1-x</sub>FeO<sub>3</sub>). Sophisticated synthesis methods in area C such as spray flame synthesis or colloid-based methods are applied to obtain phase-pure uniform nanoparticles with narrow size distribution. By using liquid-phase based methods also, the NP morphology can be controlled. The overarching aim is to establish structure-activity correlations, which are strongly influenced by the defect structure characterized in area B. For example, oxygen vacancies play a major role in the thermal oxidation of alcohols, and the oxygen evolution reaction (OER) catalyzed by the cobalt oxide NPs involves additional structural changes including the formation of hydroxides. It is the task of the projects in area A to determine the catalytic properties of the various samples. A matrix consisting of reactants to be oxidized and of oxidizing agents has been established as basis of a comprehensive comparative study.

M. Behrens, M. Muhler



Website of CRC/TRR 247



### **FIGURE 1** Concept of the comparative study in the CRC/TRR 247.

www.mrd.rub.de

M. Behrens, M. Muhler



Website of project A1 of CRC/TRR 247

#### FIGURE 1

Typical batch reactors applied in thermal liquid-phase oxidation [I].

### Thermal catalysis: activity and selectivity patterns of transition metal oxides in different oxidation reactions

Alcohols such as 2-propanol and hydrocarbons such as cyclohexene are converted in discontinuously operated batch reactors in project AI of CRC/TRR 247. Oxidizing agents are tert-butyl hydroperoxide (TBHP), hydrogen peroxide ( $H_2O_2$ ) and oxygen ( $O_2$ ). The application of the latter requires stainless steel autoclaves due to the required high-pressure conditions because of the limited solubility of  $O_2$  in water. TBHP is usually applied in organic solvents such as acetonitrile. Figure I shows typical reactors operated under atmospheric conditions (left) and high-pressure conditions (right). In these kinetic experiments, conversion and the selectivities to the various products comprising ketones, acids, peroxides, or epoxides are determined as a function of the process conditions, allowing us to derive rate laws. Mechanistic studies additionally apply in situ methods such as ATR-IR spectroscopy to identify reaction intermediates.



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### Electrocatalysis and in-depth electrochemical characterization of structureactivity and defect-activity relations

In project A2 of CRC/TRR 247 anodic alcohol oxidation and the oxygen evolution reaction (OER) are induced by applying a potential in an electrochemical cell comprising three electrodes. A suitable ink has to be applied to attach the NPs to a working electrode made of glassy carbon. As a starting point, linear sweep voltammetry and rotating disk experiments (RDE) are performed to determine the overpotential needed to achieve a certain current density. In-depth studies aim at determining the electrochemical properties of single NPs by performing nanoparticle impact measurements or by applying microelectrodes with individually immobilized NPs. Single-particle electrochemistry comprises particle-at-thestick measurements and scanning electrochemical cell microscopy (SECCM). Figure 1 shows an individual Co3O4 hexagon particle immobilized on the surface of a carbon nanoelectrode. Using a specifically designed transmission electron microscopy (TEM) holder, the particle on the nanoelectrode can be evaluated with respect to structural changes by means of identical-location TEM after challenging the catalyst particle at high electrocatalytic turnover rates.

Spectroscopic techniques such as ATR-IR and Raman spectroscopy are applied in situ to monitor reaction intermediates and structural properties, supported by identical location and liquidcell TEM studies. By combining the results of thermal and electrocatalysis with the structural characterization in area B, the analysis of the impact of the real structure on the catalytic properties is expected to lead to reliable defect-activity correlations, which have to take the dynamics of the applied cobalt oxide nanoparticles under strongly oxidizing conditions in the liquid phase into account.

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K. Tschulik, W. Schuhmann



Website of project A2 of CRC/TRR 247



FIGURE 1

 $Co_3O_4$  hexagon particle immobilized on the surface of a carbon nanoelectrode [1].

## CRC/TR 287 - BULK-REACTION: A new Collaborative Research Centre on particle systems in gaseous fluids

In 2020 a new Collaborative Research Centre started work at the Ruhr-University Bochum. In the interdisciplinary activity, researchers from the faculties of electrical engineering (Ilona Rolfes and Thomas Musch), mechanical engineering (Francesca di Mare, Martin Mönnigmann, and Viktor Scherer) and physics and astronomy (Miriam Fritsch and Ulrich Wiedner) participate. The Collaborative Research Centre/Transregio 287 BULK-REACTION explores the interaction of physical and chemical processes in reacting and moving dense particle systems passed by a gaseous fluid. BULK-REACTION combines the methods and expertise from reactive fluid mechanics with particle technology in a new multiscale approach, ranging from microscopic pores inside particles, to the void spaces between particles, up to complete systems of industrial scale. Reacting dense particle systems form the basis of a multitude of processes and are present in a wide variety of industrial sectors (e.g. for energy storage solutions; thermal use of solid biomass; treatment of bulk solids in process, chemical, pharmaceutical and food industry). These processes are indispensable for the safety of supply

with many granular products in industrialized societies. BULK-REACTION builds upon the collaboration of leading research groups in the field of the Discrete Element Method (DEM) for reactive systems in Bochum, with experts in the simulation and the experimental analysis of energy-intensive particle processes in Magdeburg.

The objectives of BULK-REACTION can be summarized as follows: First, develop new or improve existing measurement techniques to generate data from inside reacting, dense granular assemblies passed by a gaseous fluid. Second, provide measurement data (flow field, temperature and species distribution, particle trajectories) to be able to explain the phenomena in reacting granular assemblies and to validate corresponding models. Third, derive models that allow for a quantitative description of the underlying physical and chemical processes from the micro-scale (e.g. turbulent eddies, local processes within particles) up to the system scale (e. g. product quality). Fourth, develop a novel DEM model framework able to describe, spatially and temporally resolved, chemically reacting



V. Scherer



Website of CRC/TR 287

#### **FIGURE 1**

Discrete element method (DEM) simulation of a hearth furnace floor for the treatment of minerals. processes in bulk solids. This lays the ground for a technically sound design and optimization of such processes. Fifth, provide system experiments, which allow to verify that the DEM framework developed is able to correctly predict the system behavior.

BULK-REACTION will form the scientific basis to precisely predict product quality parameters, to enhance energy efficiency and to reduce  $CO_2$  emissions in important unit operations of process industries. BULK-REACTION is allocated to the Research Department Closed Carbon Cycle Economy but also closely related to the Research Department Materials Research. The material parameters (quality) of a particulate product depend on the interplay of gas and particle phase reaction.

# RUB's participation in International Max Planck Research Schools

G. Eggeler, M. Muhler

Since 2000, International Max Planck Research Schools (IMPRS) have been established by the Max Planck Society (MPG) to promote young materials researchers. Talented junior scientists can earn a doctorate degree in excellent research environments. A characteristic feature of IMPRS is a close collaboration between Max Planck institutes and universities. Shortly after the programme had been established, the Max-Planck-Institut für Eisenforschung (MPIE) launched the IMPRS SurMat in 2004, with Martin Stratmann and Gunther Eggeler as Spokesmen. Originally, SurMat stood for Surface and Interface Engineering in Advanced Materials. In its first funding phase the IMPRS SurMat was supported by the MPG, the state NRW and our university, at the time when Prof. Gerhard Wagner was our rector.

In 2004, IMPRS SurMat opened with a scientific symposium with distinguished guests from the national and international scientific community, from politics and industry. Sir Harry Bhadeshia, professor for metallurgy at the University of Cambridge, gave the keynote lecture. IMPRS SurMat started with 15 graduate students from all over the world. After they had obtained their doctoral degrees, they all found attractive positions, some of them successfully applied for academic positions in their home countries.

The IMPRS SurMat proposal was evaluated by international experts, who thoroughly considered criteria like excellence, impact, quality and efficiency of implantation. Establishing IMPRS SurMat clearly helped, when in 2006, our university successfully applied for the RUB Research School in the framework of the first German Excellence Initiative. Over the years IMPRS SurMat students participated in the Materials Days of our university and helped to make the events more colourful, lively and interesting.



FIGURE 1 Discussions between MPIE, NRW und RUB on establishing IMPRS SurMat, 2004. Participants of the opening symposium of the IMPRS SurMat in 2004.





Website of IMPRS SurMat

Over the years IMPRS SurMat has evolved, both in terms of size and focus, through three funding periods. In the last years, Prof. Dr. Jörg Neugebauer has replaced Martin Stratmann as a chairman and the IMPRS SurMat has changed focus. It is now referred to as International Max Planck Research School for Interface Controlled Materials for Energy Conversion. In its present third and final six year funding period, two Max Planck institutes (MPIE and the Max-Planck-Institut für Kohlenforschung, MPIK) and two universities (RUB and the University of Duisburg/ Essen, UDE) participate in IMPRS-SurMat.

In 2011, a new Max Planck Institute for Chemical Energy Conversion (MPI CEC) was founded in our area, with Prof. Dr. Robert Schlögl as the founding director. It was decided to launch a second IMPRS on Reactive Structure Analysis for Chemical Reactions (RECHARGE), with participation of MPI CEC and MPIK, RUB, UDE and the University Bonn. The IMPRS RECHAR-GE started in 2015 and is now in its second funding period. The spokesperson of the school is Prof. Dr. Frank Neese, who was director at MPI CEC until 12/2017, and is presently director at MPIK since 01/2018. IMPRS RECHARGE has a stronger focus on the chemical aspects of materials science and on the fundamental mechanisms of relevant energy conversion processes. Its scienitific objective is to unify the catalytic concepts towards a rational design of both homogeneous and heterogeneous catalysts. Therefore, the training program of the doctoral students



FIGURE 3 Graduation of first group of IMPRS SurMat students

2007.





ranges from advanced quantum chemical methodologies to suitable in situ spectroscopic methods. In this way, the two IMPRSs, SurMat and RECHARGE, are complementary and strongly benefit from each other.

While IMPRS RECHARGE is up and running, IMPRS SurMat now comes to an end. A new IMPRS on Sustainable Metallurgy (SusMet) is planned. The proposed new IMPRS SusMet will address and answer fundamental questions in the emerging field of Sustainable Metallurgy. Metallurgy is one of the core foundations of modern society. In the past, research in metallurgy was mainly directed towards inventing new alloys, advancing mechanical properties through microstructure adjustment and reducing costs. The huge annual production of nowadays about 2 billion tons of metallic materials is not only an engineering success story but has also become the biggest single industrial environmental burden of our generation. The present grand societal challenges in the context of sustainability, energy, transportation, health and pollution therefore require fundamental and disruptive innovations in the field of metallurgy. Key topics that need to be addressed in this context are (i) primary synthesis, which is e.g. for steels one of the largest global sources of greenhouse gas emissions, (ii) secondary synthesis (recycling), (iii) increasing operation and service lifetimes and related to this (iv) prevention and reduction of environmental induced degradation (e.g. corrosion). These challenges do not only encompass mass produced materials such as steels and aluminium alloys but also less common ones, such as copper, lithium, rare earth elements and NiTi based shape memory alloys.

FIGURE 4 IMPRS SurMat students and MRD members at RUB's Materials Day 2016.



Website of IMPRS RECHARGE



FIGURE 5 Kick-off meeting of the IMPRS RECHARGE in 2015.



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