MAPEX Bremen
Material. Process. Excellence.

03
10-2016

NEWSletter

II HIGHLIGHTS

New MAPEX Funding Lines

- Impulses for new interdisciplinary projects
- Research stays abroad for postdocs and ECIs (incoming and outgoing)
- Sabbatical support (incoming)

INSTRUMENT DATABASE

- High Performance Computing Cluster QM3

MAPEX COMMUNITY II Institutes

- Stiftung Institut für Werkstofftechnik (IWT)
- Fraunhofer-Institut für Fertigungstechnik und Angewandte Materialforschung IFAM

SCIENCE & PROJECTS II Running coordinated DFG projects

- **FOR 2213:** Nanoporous Gold
- **SFB/TR 136:** Process Signatures
- **SFB 747:** Micro Cold Forming

MAPEX Funding

All details and collection dates for proposals are available online.

www.uni-bremen.de/de/mapex > MAPEX Funding

Impulses for new interdisciplinary projects

All MAPEX members are invited to apply for funding that is especially dedicated to the initiation of new interdisciplinary collaborations between two or more MAPEX members from at least two different disciplines and groups.

Research stays abroad

MAPEX sabbatical support

The MAPEX Center for Materials and Processes invites international academics to apply for sabbatical funding to spend two to six months at the University of Bremen hosted by a research group member of MAPEX.

MAPEX Research Grants

International early stage researchers (ECIs, postdocs) are invited to apply for short-term research grants to spend a limited period of time (two weeks to two months) at the University of Bremen within the group of a MAPEX member (incoming) or at a prestigious research institutions abroad (outgoing).

MAPEX PhD Research Grants

PhD candidates of MAPEX members or from abroad are invited to apply for short-term research grants (one week to one month), within a group of a MAPEX member (incoming) or at an international research institution (outgoing).

Workshop funding

MAPEX can fund scientific workshops organized by its members and taking place in Bremen with up to 3000 Euro. A strong connection to the MAPEX research landscape should exist.

Child care during MAPEX events

To facilitate the participation of young parents at MAPEX events that last until late afternoon, we offer a child-care service. The support involves the payment of the familiar babysitter and if necessary help finding a babysitter. Please contact Hanna Lührs for more information.

Accompanying person for infants on business trips

Conference trips, journeys in order to perform special experiments, or visits to cooperation partners are an essential part of the scientific work. For parents of infants, these trips represent an almost insurmountable obstacle. MAPEX can contribute to the travel costs for an accompanying person taking care of the accompanying infant or contribute to the additional care costs at home. Please contact Hanna Lührs for more information.

Monthly Lunch Meeting

A monthly jour fixe of the MAPEX Early Career Investigators (ECI) is the informal lunch meeting, taking place every last Tuesday in the month in the Mensa. All interested scientists and PhD students are invited to get in touch with peers from different faculties and institutes. Upcoming dates online.

MAPEX SYMPOSIUM 2016

With a fantastic early-summer evening at the "Schlachte" promenade of the river Weser, the members of the International Advisory Board and the organizing committee had a perfect kick-off for the first MAPEX Symposium that took place on June 6th and 7th 2016.

The first day was dedicated to the three major fields of the MAPEX research landscape – Materials – Technologies – Methods. Nine MAPEX scientists from all career stages presented their research projects in front of the interdisciplinary audience in the well-filled Olbers-Saal in the "Haus der Wissenschaft". After the guided city-tour had to be interrupted due to a heavy thunderstorm, a nice dinner at the Restaurant Jürgenshof rounded off the day.

Cooperation projects with the industry were in the focus on the second event day, with two tandem talks given by the MAPEX Principal Investigators Prof. H.-W. Zoch (IWT) and Prof. A. Hermann (FIBRE) together with their cooperation partners Winfried Gräfen (Hanomag Lohnhärterei GmbH, Hannover) and Andre Walter (Airbus Operations, Head of Site and Plant Bremen), respectively. Before the panel meetings took place in the afternoon, a tour through the Laboratory for Precision Machining was scheduled and, as another highlight, the board members enjoyed a lunch buffet with the nice panoramic view from the top of the drop-tower.

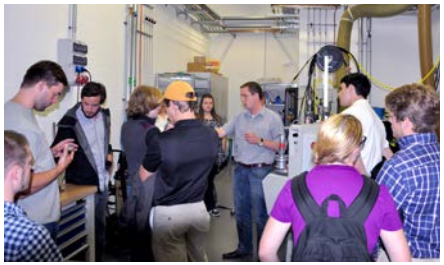
More impressions from the Symposium

www.uni-bremen.de/mapex > impressions

ENGINEERING STUDENTS FROM THE UNIVERSITY OF TENNESSEE VISITING MAPEX

A group of undergraduate students from the engineering department of the University of Tennessee (USA) and their professor visited the University of Bremen and MAPEX last June as part of their two-weeks program in Germany on "Global Perspectives on Lean, Reliability & Maintainability".

The MAPEX speaker and FB4 Dean of Studies Lucio Colombi Ciacchi and Hanna Lührs introduced them into the different courses of study within the department of production engineering and gave a brief overview of the MAPEX research activities. The highlight of their visits was a guided tour with the scientists of the Department of Welding and Allied Processes within the BIAS institute. Here our guests learned about techniques such as hybrid welding of steel, welding under vibrations, high-speed laser-drilling as well as laser metal deposition, selective laser melting and thermal rod end melting. As the final activity before getting on the bus back to Hamburg, the International Office organized a walking tour over the campus of the university.



MAPEX CALENDAR

25 October 2016 MAPEX lunch meeting for Young Scientists
12:30 Mensa

31 October 2016 MAPEX General Assembly
14.00-16:00 LION

29 November 2016 MAPEX lunch meeting for Young Scientists
12:30 Mensa

December 2016 Young Scientist Visit to OHB System AG

More events, seminars, and talks related to MAPEX topics:
www.uni-bremen.de/mapex > events > calendar

Universität Bremen*

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* This project is funded by the German Excellence Initiative.

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Link to online version of newsletter: *www.uni-bremen.de/mapex > news > newsletter*

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MAPEX COMMUNITY
Institutes

Universität Bremen

II STIFTUNG INSTITUT FÜR WERKSTOFFTECHNIK

IWT
Stiftung Institut für Werkstofftechnik Bremen

Scope of Research: The IWT develops technologies for the future in metalworking. The comprehensive know-how and the broad range of technical equipment are put forward with the aim of solving particular problems in material improvement, material treatment and metalworking. The IWT is a Bremen institution with a rich research tradition of more than 60 years. The overall objective is to carry out multidisciplinary basic and applied research in the field of metalworking and related technologies covering entire process chains of high strength structural metallic materials. The IWT is the only research centre in Europe with three joint disciplines of materials science, process engineering and manufacturing technologies as equal-ranking divisions under one roof. Key aspects are the research fields, "heat treatment and surface technology", "hybrid lightweight structures", "distortion engineering", "ecologically efficient and high-precision machining technologies" as well as "particle technologies including sprayforming".

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Badgasteiner Strasse 3 II 28359 Bremen
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iwt@iwt-bremen.de II www.iwt-bremen.de

Facts and Figures

- Founding Year: 1950 (former Institut für Härtereitechnik – IHT, since 1986 IWT)
- Personnel: Approx. 160 Employees
- Main Business Areas: Automotive, Aviation, Heat Treatment, Machining and Particle Technology

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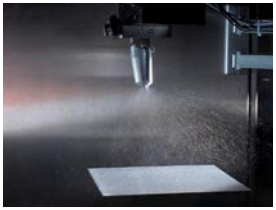
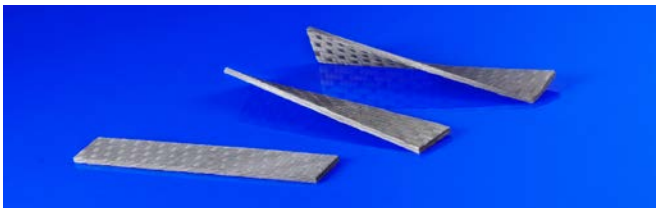
|| FRAUNHOFER INSTITUTE FOR MANUFACTURING TECHNOLOGY AND ADVANCED MATERIALS IFAM

Fraunhofer IFAM

Founded in 1968 and integrated into the Fraunhofer-Gesellschaft in 1974, Fraunhofer IFAM is one of the most important research institutions in Europe for adhesive bonding technology, surfaces, shaping, and functional materials. At our institute's five locations – Bremen, Dresden, Oldenburg, Stade, and Wolfsburg – we put our central principles into practice: scientific excellence, a focus on the application of technology, measurable utility for customers, and ensuring the highest quality.

Our 580 employees, working in 24 departments, combine their broad technological and scientific knowledge and expertise into seven core competencies: Powder Technology; Sintered, Composite, and Cellular Metallic Materials; Adhesive Bonding Technology; Surface Technology; Casting Technology; Electrical Components and Systems; and Fiber Reinforced Plastics. These core competencies - both individually and in combination with each other – are not only the basis of our strong position in the research market but also of future-forward developments that will be useful for society.





left) Investigation of the wetting properties of surfaces using the aerosol wetting test;
right) Strong and flexible – malleable lightweight construction materials

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Facts and Figures
- Founding Year: 1968
- Personnel: 580 Employees

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SCIENCE & PROJECTS
Large-Scale Research Projects

Universität Bremen

II RUNNING COORDINATED DFG PROJECTS

In the past years, the University of Bremen and the cooperating external institutes located on the university campus have established themselves as a world-leading group of researchers in the field of materials-oriented development of processes, and at the same time of process-oriented development of materials, with a special focus on metals, nanoparticulate materials, carbonreinforced composites, semiconductors, and porous ceramics. The close connection between achieving novel properties and establishing innovative processing routes in materials engineering, making use of chemical/physical analyses and investigation methods, concurrently with mathematical and physical modelling at multiple scales, is best exemplified by the ten running coordinated DFG projects.

Collaborative Research Centers (SFB)

- SFB 747: Micro Cold Forming
- SFB TR 136: Process Signatures
- SFB 1232: Farbige Zustände (newsletter 02)

Research Units

- FOR 1224: Schwarz-Silber (newsletter 04)
- FOR 1845: Ultra-Precision High Performance Cutting (newsletter 04)
- FOR 2213: Nanoporous gold

Priority Program

- SPP 1676: Dry Metal Forming (newsletter 04)

Research Training Groups

- GRK 1860: MIMENIMA (newsletter 04)
- GRK 2247: Quantum Mechanical Materials Modelling – QM³ (newsletter 02-2016)
- GRK 2224: π^3: Parameter Identification – Analysis, Algorithms, Implementations (newsletter 02)

II RESEARCH UNIT 2213: NANOPOROUS GOLD - A PROTOTYPE FOR A RATIONAL DESIGN OF CATALYSTS

NAGOCAT FOR 2213

Nanoporous gold is a relatively new catalyst with great potential in heterogeneous gas and liquid phase catalysis and electrocatalysis. It is a sponge-like material with ligaments and pores in the range of a few 10 nm. Its catalytic properties are influenced by traces of a second metal and the nanostructure. The DFG research unit NaGoCat aims at elucidating these factors on different length scales from the atomistic level (active sites for adsorption and reaction) up to the mesoscopic level (transport of the reactants by diffusion).

This interdisciplinary effort is only possible by bringing together the expertise of eight groups from four different universities in northern Germany (Oldenburg, Bremen, Hamburg-Harburg, Berlin), contributing experimental as well as theoretical expertise in chemistry, materials sciences, and physics. Three areas are covered in the unit: material preparation and characterization, gas phase catalysis and liquid phase catalysis/electrocatalysis. Bringing together basic insight from theory and fundamental research as well as experiments on nanoporous gold under ambient/working conditions, the unit aims at exploring its catalytic properties with special attention to the impact of varying chemical and structural features of the surface as well as the scale and geometry of the pores on the activity and selectivity for the oxidation of primary alcohols, an industrially relevant reaction.

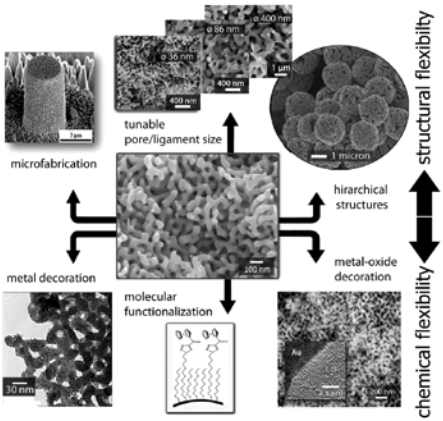
Research Unit 2213: Nanoporous gold - A prototype for a rational design of catalysts

Funding: 2014 –

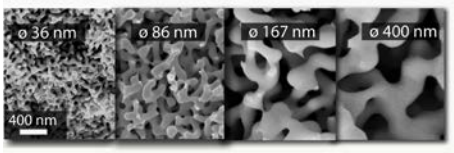
Speaker: Marcus Bäumer

Subproject leaders from MAPEX: Marcus Bäumer, Andreas Rosenauer and Arne Wittstock

Website: www.nagocat.uni-bremen.de



Nanoporous gold as a flexible functional material (Reproduced/Adapted from Wittstock et al., Nanoporous Gold: from an Ancient Technology to a Novel Material, RSC, 2012, p. 250).



Coarsening of the pore structure of npAu upon annealing (note similar scale bars).

COLLABORATIVE RESEARCH CENTER 747: MICRO COLD FORMING - PROCESSES, CHARACTERIZATION, OPTIMIZATION

The Collaborative Research Center 747 „micro cold forming“ (German: Sonderforschungs-bereich 747 “Mikrokaltumformen”) is a 12 year long basic research project financed by the Deutsche Forschungsgemeinschaft. It is located at University of Bremen since 2007.

Aim of the SFB 747

Central concern of the Collaborative Research Center is the provision of methods and processes for a systematic design of reliable micro cold forming processes with focus on its implementation in industrial applications of metallic micro components produced with lot sizes greater than one million pieces.

Expertise areas of the SFB 747

An effective treatment of technical issues of micro metal forming requires an accurate consideration of basic material properties, their modifications owing to controlled process impacts, the resulting component properties and process design. Approximately 70 scientists and technicians from the disciplines of engineering, physics, materials science, and mathematics rise to these challenges in the expertise areas micro forming processes, tools, materials, properties and process design.

Industry network

During its activities the Research Center is attended by a network of industry partners, which is regularly informed about the most recent results. Mutual exchange within the network as in the annual meeting provides a basis for corporate projects aiming at a transfer of scientific achievements into industrial applications.

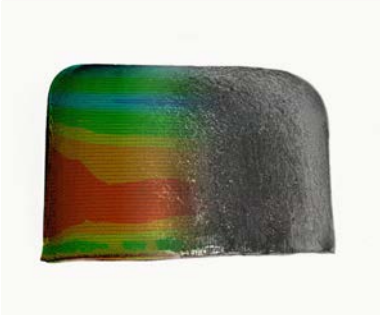
Collaborative Research Center 747:
Micro Cold Forming - Processes, Characterization, Optimization

Funding: 2007 - 2018

Speaker: Frank Vollertsen; **Vice Speaker:** Peter Maaß; **Administration:** Sybille Friedrich

Subproject leaders from MAPEX:
Ralf B. Bergmann, Ekkard Brinksmeier, Bernd Kuhfuß, Peter Maaß Alfred Schmidt, Kristen Tracht, Frank Vollertsen, Hans-Werner Zoch

Website: www.sfb747.uni-bremen.de



Metallic Microcup superimposed with FEM-Simulation.

II TRANSREGIONAL COLLABORATIVE RESEARCH CENTRE 136: FUNCTION-ORIENTED MANUFACTURING BASED ON CHARACTERISTIC PROCESS SIGNATURES

The generation of well-defined geometrical properties in machining processes is state of the art in industry. This is not true for chemical and physical material properties of the workpiece surface layer. However, these properties are of main importance regarding the functional performance of the part. The reason is that even today a fundamental understanding of the basic mechanisms leading to material alterations in machining processes is still missing. The transregional Collaborative Research Centre 136 (CRC 136) "Process Signatures", a collaboration of the University of Bremen, the RWTH Aachen University, and the Oklahoma State University, established in 2014 is aiming exactly at this knowledge gap.

The work within the transregional CRC 136 focuses on identifying the quantitative dependencies of state variable changes (e.g. residual stresses, phase composition, chemical composition) on the internal material loading state of the workpiece during the manufacturing processes e.g., the time-dependent stress-strain state, temperature field and spatially varying chemical potential. By means of Process Signatures it will be possible to describe manufacturing processes in a unified way for the first time. The long-term objective of the research work is to solve the so-called inverse problem of manufacturing technology: By utilising Process Signatures it will be possible to select the necessary manufacturing processes, the corresponding parameters and the subsequent application of further machining processes based on previously defined chemical and physical material properties of the workpiece surface layer.

Transregional Collaborative Research Centre 136: Function-Oriented Manufacturing Based on Characteristic Process Signatures

Funding: 2014 – 2017 (first funding period)

Speaker: Ekkard Brinksmeier; **Vice Speaker:** Fritz Klocke (RWTH Aachen); **Executive Manager:** Jens Sölter

Subproject leaders from MAPEX: Ekkard Brinksmeier, Carsten Heinzel, Walter Lang, Daniel Meyer, Jens Sölter, Frank Vollertsen, Hans-Werner Zoch

Website: www.prozesssignaturen.de

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INSTRUMENT DATABASE
High Performance Computing Cluster QM3

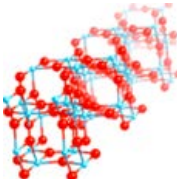
Universität Bremen

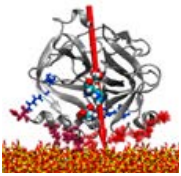
BREMEN CENTER FOR COMPUTATIONAL MATERIALS SCIENCE (BCCMS)

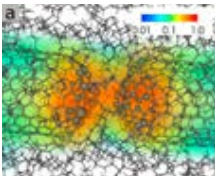
BCCMS Bremen Center for Computational Materials Science

The Bremen Center for Computational Materials Science – BCCMS was founded in 2006 as an interdisciplinary research center of the science and engineering faculties at the University of Bremen.

The available materials and process simulation expertise ranges from many-body electron theory (Prof. Tim Wehling), quantum mechanical materials modelling (Prof. Thomas Frauenheim), atomistic and mesoscopic coarse-grained (CG) modelling (Prof. Lucio Colombi Ciacchi) up to microstructure evolution modelling (Prof. Vasily Ploshikhin). The aim is to merge the multi-scale expertise of different fields in computational materials science, life science, and engineering in order to address urging questions related to future materials development in renewable energy, safe environment, transportation, and health. The new computing cluster will be of special benefit for the twelve PhD students within the recently established Research Training Group 2247 "Quantum Mechanical Materials Modelling QM³" that is coordinated by the two MAPEX members Thomas Frauenheim and Tim Wehling.







From left to right:

1) Atomic structure of Fe-hydrogen complex adsorbed on a Pt(111) surface.

2) Fundamental electronic properties of TiO_2: bulk, surfaces, interfaces, nanostructures.

3) Protein adsorption on solid surfaces studied with quantum mechanical and classical Molecular Dynamics.

4) Prediction of electrical properties of carbon-nanotube- reinforced polymers.

Due to a number of significant advances in first-principles quantum-mechanical, classical atomistic, coarse graining, and finite element calculations over the past decade, coupled with the highly improved efficiency of software and computer architectures, it is only now becoming possible to investigate materials at a very high level of theory and under operational and loading conditions, fully taking into account atomistic and electronic details with reliable experimental accuracy.

|| HIGH PERFORMANCE COMPUTING CLUSTER QM3

01 || General Information

Keywords: quantum mechanics, molecular transport, electronic conductivity, DFT, materials properties, nanoscale simulations, electronic correlation and transport, low-dimensional systems, molecules at surfaces

Categories

- Computing

Main application: theoretical physics, chemistry and materials science on atomistic scale including electronic degrees of freedom.

Year of Fabrication: 2016

Manufacturer: Megware Computer GmbH

02 || Specifications

- 109 compute nodes
- 20xE5-2660v3 cores per node, 2180 total cores
- 128 GByte RAM per node
- Intel OmniPath high-performance interconnect
- BeeGFS scratch storage with 175 TByte of space
- Operating System CentOS 7

03 || Contact

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Principal Investigator: Thomas Frauenheim