TECHNISCHE UNIVERSITÄT DRESDEN

JAN EVANGELISTA PURKYNĚ UNIVERSITY IN ÚSTÍ NAD LABEM

Proceedings of the 1st Joint PhD Conference on Material Science:

Biologization
Nanotechnology
Simulation

from 27.6. - 1.7.2022 in Dresden/ Germany and Usti n. L. / Czech Republic

ed. by Ute Bergmann, Theresa König

Europäische Union. Europäischer Fonds für regionale Entwicklung.
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1 Introduction

Materials scientists from Ústí nad Labem and Dresden met in June of 2022 for the first joint PhD Conference on Material Science, with the special focus on biologization, nanotechnology and simulation. The conference aimed to encourage interdisciplinary exchange between Čzech and German research institutes and promote transnational cooperation on an international level along the Saxon- Čzech border. Due to the restrictions caused by the corona pandemic, several attempts were necessary before the conference, which was first planned in 2020, could finally take place for the first time in 2022. The conference could take place in presence, which was seen as a big plus by all participants, especially as it was the first meeting in this German - Čzech context for most of the participants.

The attending scientists (about 60) met at the Institute of Material Science of TU Dresden in Germany for the first half of the week before the conference moved to the faculties of Science and Environment of the Jan Evangelista Purkyně University UJEP in Ústí nad Labem in Čzechia. The organized activities ranged from scientific presentations of current PhD projects and research topics, lab tours in the participating institutions, come-together events such as a guided tour at the dye collection of the TU Dresden and a hiking trip to Bohemian Switzerland. The conference was funded by INTERREG VA Saxony - Čzech Republic - a cooperation programme of the Elbe/Labe region. All participants - PhD students, scientists and staff members of the participating institutions - enjoyed this opportunity to build individual and new contacts, exchange information on current research topics and methods, find starting points for future collaborations between the different research areas and institutions and also discuss the similarities and differences between the German and Čzech research landscape.

The purpose of this brochure is to present the institutions with their special topics and laboratories and to present current research topics - on the base of the presented PhD projects.

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1.1 Committees

Scientific Organizing Committee

Technische Universität Dresden:

- Dr. rer. nat. Joerg Opitz, Head of Department: Bio- and Nanotechnology, Head of Research Field Biomedical Engineering in Fraunhofer Institute for Ceramic Technologies and Systems IKTS
- Dr. Ing. Ute Bergmann, Chair Biomaterials, Head of Group Corrosion and Surfaces, Institute of Material Science, TU Dresden

Jan Evangelista Purkyně University in Ústí nad Labem

- Prof. RNDr. Pavla Čapková, DrSc., Deputy Head of Centre for Nanomaterials and Biotechnology; Nanotechnology
- doc. RNDr. Michal Varady, Ph.D., Dean of Faculty of Science; Department of Physics
- Mgr. Jan Malý, Ph.D., Head of Centre for Nanomaterials and Biotechnology
- doc. RNDr. Filip Moučka, Ph.D., Associate Professor; Department of Physics
- prof. Ing. Zdeňka Kolská, Ph.D., Centre for Nanomaterials and Biotechnology
- Ing. Jiří Orava Ph.D., Assistant Professor; Materials Science

Local Organizing Committee

- Ing. Petr Lauterbach, Fac. of Science, Jan Evangelista Purkyně University in Ústí nad Labem
- Ing. Kateřina Stehlíková, Assistant of Development Department, Fac. of Science, Jan Evangelista Purkyně University in Ústí nad Labem
- Dipl.-Ing. Gritt Ott, CIMTT, TU Dresden
- Theresa König, Sc. Assistant, Fac. of Mech. Engineering, TU Dresden

2 Presentation of the participating institutes and chairs

2.1 Jan Evangelista Purkyně University in Ústí nad Labem

JAN EVANGELISTA PURKYNĚ UNIVERSITY IN ÚSTÍ NAD LABEM

The university has adopted the name of a renowned North-Bohemian native of Libochovice (1787-1869), Jan Evangelista Purkyně, who is consic such as biology, embryology, histology, modern pharmacology, comparat Purkyně ranked among the world´s most outstanding physiologists.

Just as well-rounded a personality Purkyně in his time was, the university too, in these days, offers a wide range of study programmes and specialisations (55 programmes and 173 specialisations) covering broad areas of human activities. With such a wide range of programmes, the university has become attractive for the resent generation of young people.

The university is a state-of-the-art scientific, pedagogic, cultural and educational center of the Ústí nad Labem region.

The university educates a number of students exceeding 10 000 and employes about 900 members of staff.

The university proudly takes credit for the municipality of Ústí nad Labem and contributes significantly to the development of the region.

UJEP university dates back to 1991, and is currently known as the umbrella term for 8 faculties. These are the:

- Faculty of Art and Design
- Faculty of Arts
- Faculty of Education
- Faculty of the Environment
- Faculty of Health Studies
- Faculty of Mechanical Engineering
- Faculty of Science
- Faculty of Social and Economic Studies

Find more information on the website: **https://www.ujep.cz/en/about-ujep**

2.1.1 Faculty of Science

JAN EVANGELISTA PURKYNĚ UNIVERSITY IN ÚSTÍ NAD LABEM
Faculty of Science

The Faculty of Science at Jan Evangelista Purkyně University in Ústí nad Labem is the second youngest faculty of the university. Its history goes back to the spring of 2005 when the Institute of Science was established at UJEP. On the 4 November 2005, the Institute was transformed into Faculty. Since that time the Faculty of Science has firmly established itself among the other Faculties of Sciences in Czechia.

2.1.1.1 Parts of the Faculty of Science

- Department of Biology
- Department of Physics
- Department of Geography
- Department of Chemistry
- Department of Informatics
- Department of Mathematics
- Centre for Nanomaterials and Biotechnologies
- Centre for Promotion of Science Education

In the framework of the departments, the Faculty offers over 17 study fields and combinations at three levels, both as full-time and combined study.

Since 2020, we can be proud of the new building, which is the largest campus building. It is the seat of the Faculty of Science, the Faculty of the Environment and is equipped with the latest instruments.

Main faculty building – Centre for Natural Sciences and Technologies

Website: **https://prf.ujep.cz/en/**

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The mission of the Faculty of Science is to encourage learning and develop knowledge in the fields of natural sciences. Its aim is to boost science and research base of UJEP in the field of natural sciences and acquire greater integration in the European research space and international cooperation network. The next task of the Faculty of Science is to provide higher education at all the three levels (Bachelor, Master, PhD.) both in natural sciences and close technical fields, and also for teachers of natural sciences subjects for the second stage of basic schools and for secondary schools. The faculty prepares graduates in such way that they can find good employment at the employment market, and at the same time, are able to engage in science research.

In the field of science and research, the faculty mainly focuses on computer physics, computer methods and simulations, the problem of methodology of molecular simulation and their application for problems of physics, chemistry and chemical engineering, modelling of energy processes in solar atmosphere with orientation towards eruption physics, further towards the physics of plasmas, plazmochemistry, physics of thin layers and surfaces, research of electrochemical biosensors for environment analysis, microbiology and biology of plants and animals, application geography, environmental geography, country ecology, country synthesis, country planning and instrumental methods in analytical chemistry.

2.1.1.2 Department of Physics

DEPT. OF PHYSICS

The role of the Physics Department is to educate and train students in Bachelor's of Science, Master's of Science and PhD study programmes, and to promote scientific and research activities and cooperation with companies and specialized institutes not only in Czechia but also abroad.

Website: **https://www.physics.ujep.cz**

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Education provided by the department focuses on preparation of future experts in computer modelling, nanotechnologies and preparation of future teachers of physics. At the department, students can study a Bachelor's single-subject programme specialized on computer modelling or experimental methods in physics. Computer modelling can be also studied in the recently innovated study programme Computer Modelling in Science and Technology. In a two-subject Bachelor's programme, students can study physics in combination with another subject. The department also provides training in the multidisciplinary Bachelor's programme Applied Nanotechnology in cooperation with other parts of the faculty. Students can proceed with the MSc programmes Applied Nanotechnology or Computer Modelling in Science and Technology. They can further extend and deepen their knowledge and scientific abilities in PhD study programmes. The study programme Teaching of Physics for Secondary Schools prepares future teachers.

Scientific and creative activity of the department is realized in several fields. In the field of nanotechnology, the research focuses on development of new materials and nanomaterials with the application of plasma technologies. In the field of computer modelling, computer methods and simulations are used for a wide range of problems, from the development of new materials, chemical engineering, processes in the solar atmosphere, to prediction of structures and properties of biomolecular systems. In the field of teaching physics, the research is focused on evaluation of physics education at primary schools, formation of exercises and tests and development of pupils' scientific thinking.

Employees of the department are involved in a number of national and international teams and projects. Students of the MSc and PhD programmes are also successfully involved in scientific and research activities, they can work in fully equipped laboratories under the supervision of experienced department employees. The department offers a wide range of study and work visits, which allows students to gain experience in companies and research institutes not only at universities in Czechia but also abroad.

The department offers its research services in the following fields:

- Nanotextiles for antibacterial air filtrations
- Nanoporous Polymer Membranes Prepared by Electrospinning

- Computer modeling and high-performance computing
- Computer design of nanomaterials
- Complex Services In Plasma Technologies
- Polymeric Nanofiber Membranes for Specific Functions
- Antimicrobial Nanofiber Membranes
- Ion Beam Characterization and Synthesis of Nano and Microstructures Collaboration with NPI CAS

2.1.1.3 Department of Biology

Since its establishment in 2004, the mission of the department has been to educate students of biology teaching in combination with other natural sciences and humanities within the Faculty of Education of UJEP. At present, the department within the Faculty of Science allows, in addition to the above fields, to study bachelor's single-subject study of biology in full-time and part-time, bachelor's two-subject study in full-time and part-time form (B.S. Degree), master's follow-up single-subject and two-subject study of biology in full-time and part-time form (title MSc).

In the field of teaching and education as well as in the field of science and research, we cooperate with leading national institutes of the Academy of Sciences, Masaryk Hospital in Ústí nad Labem, the Zoo in Ústí nad Labem and foreign institutes (e.g. Faculty of Biology in Łódž or the Technical University in Dresden).

The background of the department consists of a complex, which includes two buildings ("old building" and CBEO) with classrooms and laboratories, an educational botanical park, two greenhouses with a total area of 422 m2 and a separate state-of-the-art biotechnology workplace (CPTO). The educational botanical park and greenhouses provide facilities for teaching students, but also serve as an educational centre for schools and other institutions in the Ústí region. Staff and students prepare and implement several attractive events for the public. These include, for example, the Summer Schools, traditional exhibitions such as Tropical Orchids and Carnivorous Plants, Cactuses and Succulents or botanical competitions. Up to 2,500 visitors come to the complex every year.

It is important for us to create a friendly atmosphere in a pleasant environment not only for study, but also for relaxation.

Website: **https://prf.ujep.cz/en/department-of-biology**

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2.1.1.4 Centre for Nanomaterials and Biotechnology (CENAB)

The mission of the research centre is to carry out basic and applied research in the areas of preparation and application of nanomaterials of synthetic and biological origin in environmental protection, health and medicine. We study the interactions of nanomaterials with biological models at various levels of complexity, and realize the development of microfluidic devices for applications in biology, biotechnology and medical diagnostics. We are an interdisciplinary team that integrates experts in the fields of physics, chemistry, biology and computer modelling, thus creating a shared interdisciplinary research platform of the Faculty of Science, UJEP. We are members of a consortium of Large research infrastructure NanoEnviCz, which brings together nanotechnology research institutes in Czechia focused on nanotechnologies for environmental protection and sustainable development. We cooperate with research institutions in Czechia and abroad and industrial partners.

The research is connected with education through the study programme “Applied Nanotechnologies” in all three levels: bachelor’s, master’s and doctoral, as well as with the study programme “Biology”.

Website: **https://cenab.ujep.cz/cs/**

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Current research topics:

- Preparation and characterization of new materials for tissue engineering
- Research of nanofiber membranes for antimicrobial nanofiltration
- Development of nanocomposite membranes degrading dangerous toxic pollutants
- Development of a new generation of organic / inorganic materials for CO2 detection, capture and utilization
- Exosomes as natural nanovesicles in intercellular communication and the study of their use for drug delivery into cells
- Biophysical studies of the interaction of nanomaterials with biological models (liposomes, proteins, nucleic acids)
- Study of cytoskeletal properties
- Development of so-called organs on a chip for simulation of tissue barriers and 3D cell culture
- Development of microfluidic diagnostic devices / biosensors for the detection of tumor markers

2.1.1.5 Laboratories of Faculty of Science

Laboratory for the preparation of nanofibers

In this laboratory, it is possible to create and modify nanofiber polymeric materials using needle electrospinning methods. The device is also equipped with an air-conditioning chamber, which allows the preservation of reproducible conditions during the preparation of nanofibers. There are also devices for testing the water and air permeability of nanofiber and other textile membranes.

Surface analysis laboratory

SurPASS and SurPASS3 allow direct analysis of the zeta potential at the phase interface and provide surface charge information. They can measure nanofiber or powder samples. LiteSizer is used to characterize nanoparticles and microparticles, to measure particle size through dynamic light scattering (DLS). Also for measuring zeta potential and measuring molecular weight and refractive index. Using the Nova 3200, it is possible to determine the surface size (using the BET isotherm) or to measure the pore volume and pore size distribution (using the adsorption and desorption isotherms).

Laboratory of XRD and XRF X-ray methods

The X-ray fluorescence spectroscopy (XRF) method allows the determination of the concentration of elements in various matrices in the F-U range in concentrations from ppm to 100%. It is relatively fast and non-destructive. The X-ray diffraction (XRD) method allows the determination of the crystal structure of materials. That is, how the individual elements are arranged in the crystal sample. Furthermore, it is also possible to determine the size of the primary crystallites, the ratio of the individual crystalline phases in the sample. The method is non-destructive, the sample can be used repeatedly.

Laboratory of plasma technologies

The equipment of this laboratory is used to create various types of functional thin nanolayers that improve the properties of the substrate. Thin nanolayers are deposited in plasma under different deposition conditions and unique properties can be achieved (hardness, abrasion resistance, chemical stability at high temperatures, transparency at the same time as electrical conductivity, etc.)

XPS and AES surface analysis laboratory

The surface composition can be analyzed using X-ray photoelectron spectroscopy (XPS) to a depth of several nm, including the possibility of analyzing the binding energies of elements - ie determining the types of chemical bonds and states of elements. This method is very suitable for the study of surface modification in the creation of new functional nanolayers or or functional surfaces used in applications. The analysis can be supplemented by Auger electron measurement (AES) with direct surface mapping and thus create chemical maps of surfaces (elements, chemical bonds). It is also possible to purposefully modify the surfaces of ion beams with the possibility of cleaning the surfaces or their physico-chemical modification directly in the device.

Laboratory of Transmission Electron Microscopy

The laboratory is used to analyze the nanostructure of nanomaterials and biological samples of various natures using transmission electron microscopy.

Laboratory of Molecular Biology and Genetics

The laboratory is used for the purpose of isolation and analysis of biomolecules and organelles by a number of techniques, such as ultracentrifugation, electrophoresis or RT-qPCR.

Laboratory of microscopic techniques

The laboratory has two inverted fluorescence microscopes and one confocal microscope, which allow monitoring of experiments, including time-lapse records.

Tissue Techniques Laboratory

Highly controlled environment for working with a wide range of tissue cultures. Room equipment extends from incubators, through the freezer box, flowboxes to flow cytometers.

Cleanroom Laboratory / Microfluidics Laboratory

The laboratory enables the preparation of fine structures by a number of microfabrication techniques without the risk of contaminating the samples with dust particles. The laboratory also has instrumentation for the analysis of prepared structures, such as a scanning electron microscope.

Laboratory of Biophysics and Nanobiotechnology

In the laboratory, microstructures are prepared by the method of reactive ion etching and serve as a background for the assembly of microfluidic systems. Furthermore, the laboratory has a number of biophysical methods for the characterization of nanoparticles and their interactions with biological objects.

Laboratory of Model Organisms

The laboratory is equipped for breeding and experimental use of the model organism Danio rerio.

2.1.2 Faculty of Environment

JAN EVANGELISTA PURKYNĚ UNIVERSITY IN ÚSTÍ NAD LABEM
Faculty of the Environment

Jan Evangelista Purkyně University in Ústí nad Labem (UJEP) was established in 1991 with the Faculty of Environment (FŽP) among the founding faculties – it is the oldest environmentally-oriented faculty in the Czech Republic. The main impulse for the faculty establishment was the catastrophic state of the landscape and environment in the region originating from vast surface brown coal mining, its burning in non-desulphurized coal power stations as well as related social, societal and economic consequences. Thus, the initial mission of the faculty was to prepare new experts capable of understanding the environment in its complexity, capable of organizing landscape reclamation and ecosystem restoration. Throughout its 30-years history, however, research areas have been growing wider together with research capacity and study programmes. Key milestones are summarized in the *Table 1*.

Table 1: Establishment of Faculty of Environment

Year	Milestone
1991	Founding of the Faculty of Environment, BSc. programmes only (Ecology and Environmental Protection).
1996	First master programmes (Landscape Reclamation, Waste Management)
2010	First PhD programme (Environmental Analytical Chemistry), new master programme (Environmental Analytical Chemistry and Toxicology)
2016	Faculty became part of the research infrastructure NanoEnviCZ (Nanomaterials and Nanotechnologies for Environment Protection and Sustainable Future, nanoenvicz.cz)
2019	New study programmes (BSc. – Applied geoinformatics, MSc – Environmental technologies, Ph.D. – Environmental chemistry and technologies)
2020	Moving of the faculty to the new building Centre for Natural Sciences and Technologies

The faculty currently has about 280 students at bachelor, master and PhD programmes and 64 staff members. The faculty continuously reflects the needs of modern society and just recently expanded its research interest into the areas of green materials, materials for low-energy-consumption electronics, and materials for optical sensing by hiring new members of staff.

The building of the faculty of science in Ústí n. L.

Currently, the faculty research is carried out in the following areas:

- Environmental analytical chemistry (pollutants in different environments, speciation, transformation products…)
- Materials for environmental applications (reactive and functionalized sorbents, photocatalytic materials…)
- Geographic information systems for environment monitoring (mapping, data processing…)
- Environmental biotechnologies (waste-water treatment, bioremediations, phytotechnologies…)
- Ecology, landscape and climate (biodiversity and ecosystem services in the changing world, post-mining areas reclamation…)
- Waste and circular economy (materials and chemical recycling, thermolytic processes, ecotoxicity and risk assessment…)

Examples of recent achievements:

- The faculty participated in the digitalisation of cultural and natural monuments in the region which contributed to the listing of the Erzgebirge/Krušnohoří mining region into UNESCO world heritage in 2019. The faculty runs a server http://oldmaps.geolab.cz/ which provides digitalized historical maps starting from the 18th century and which can be used for example for the reconstruction of landscape changes.
- In 2017, PhD student Daniel Bůžek received the Jean Marie Lehn prize for chemistry.
- Between 2016-2021, the faculty led the international project *G4687 New Phytotechnology for Cleaning Contaminated Military Sites* supported by NATO Science for peace and security programme. The project was aimed at the research of second-generation biofuel crops for phytomanagement of contaminated post-military sites.
- In 2021, the faculty became a part of an international consortium resolving the project TH76030002 Green Ultrafiltration Water Cleaning Technologies (GreenWaterTech) supported from the Aquatic Pollutants call (H2020). The project aims to develop a new modular concept of water purification using novel porous nanomaterials and nanozymes.
- Between 2017-2020 together with Cottex Trade company the faculty participated in the development of new technology for the recovery of ultrapure zinc from zinc waste.

The Faculty of Environment has comprehensive laboratory capacities (waste processing, remediation, ecology, ecotoxicology-GMO, chemistry, geology, pedology…). Significant capacity is devoted to analytical chemistry (HPLC-DAD, HPLC-MS/MS, GCxGC-qTOF-HRMS/FID, ICP-OES, ICP-MS, portable XRF, microwave decomposition, QUERChEs, advanced separations…). Part of the laboratory capacity is separated into centres, especially CADORAN (Centre for advanced organic analyses – offers) and CPST (Center for advanced separation techniques). These support the research and also carry out commercial activities. The faculty and their members closely collaborate with the Czech Academy of Sciences in terms of teaching/training new students and sharing research facilities. The faculty is also a member of a Czech large research infrastructure called NanoEnviCz (https://www.nanoenvicz.cz/en) which provides the faculty with access to the latest and advanced experimental facilities. Close collaboration in research activities is also developed with industrial partners. The faculty is a member of cluster WastEn (https://wasten.cz/en), the organization associating Czech companies and leading research organizations in the field of technologies for the treatment of municipal and industrial waste. It is also part of Consorcium 3U (Unipetrol-UniCRE-UJEP) oriented on research and application of chemical processes for transformation of waste materials to “green chemicals”, and Czech Association of Circular Economy (http://www.caobh.cz/). In the field of ecology, the faculty members participate for example in activities of the Czech Society for Landscape Ecology (http://www.iale.cz/en/).

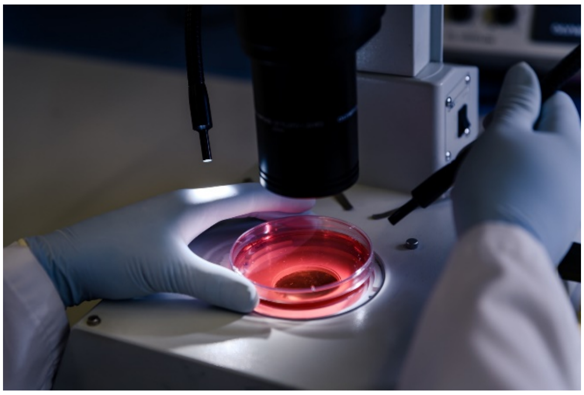
2.1.2.1 Laboratories of the Faculty of Environment

Environmental Analytical Chemistry

Environmental analytical chemistry presents the backbone of our research and it occupies the largest laboratory space.

Environmental Sampling

Faculty is equipped for terrain sampling of soils, waters, sediments (including an on-boat sampling of lakes and dams bottoms), wastes, air (including the development of on-drone air samplers), wood and others.



Portable Terrain Analyzers

The faculty possesses several portable measuring devices for direct rapid terrain measurements. These include portable XRF for detection of solid materials elemental composition, multimeter of water parameters (pH, O2, conductivity), RemScan for direct measurement of petroleum contamination in soil or Raman-spectrometer for identification of liquid samples. Related research includes analyses of sedimentary archives, pollution monitoring of soils and waters, remediation studies and others.

Environmental Sample Processing

Environmental samples can be processed by various decomposition techniques (including the rapid microwave decomposition) and separation techniques (such as filtration, concentration, column purification, QuEChERS) before final analysis. Research activities include processing of contaminated water, sediments, soil, wood, wastes and other samples.

Instrumentations for Analyses

Faculty possesses the latest advanced analytical instrumentation such as HPLC-MS/MS, HPLC-DAD, GCxGC-qTOF-HRMS/FID, GC-MS, GC-FID, ICP-OES, ICP-MS, automatic titrator, TOC and TN analyser and others. Research activities include the determination of various pollutants and their degradation products (aliphatic and aromatic hydrocarbons, halogenated compounds, pesticides, analyses of pyrolytic oils and chars, analyses of water parameters, analyses of phospholipid fatty acids and many others).

CADORAN – Centre for Advanced Organic Analyses

The laboratories are primarily equipped for the determination of trace concentrations of organic pollutants, such as pesticides, drugs and their residues, PAH, PCB and OCP. These substances are determined either in liquid matrices or solid matrices (soil, sediments). CADORAN laboratory also offers the analysis of acrylamide in water and food. Most determinations are accredited. CADORAN is equipped with modern instruments for the analysis of liquid and solid samples in the environment, for example, LC 1290 Infinity II with mass detector 6495 QQQ (Agilent Technologies), GC 7890 with mass detector 7000D (Agilent Technologies), Homogenizer 1600 miniG (SpexSamplePrep) for preparation of extracts using the QuEChERS, TOC analyzer (SKALAR), XRF spectrometer (BAS) and Raman spectrometer (Thermo).

CPST – Center for Advanced Separation Techniques

Main research and service activities of the Centre for Advanced Separation Techniques (CAST) include the development of new analytical methods with a special focus on characterization and identification of unknown substances in products from advanced chemical technologies for transformation of waste to “green chemicals”. Furthermore, CAST provides the analysis of samples from the environment and technological processes, preparation and testing of new special sorbents for environmental applications. CAST is equipped with the most sophisticated instrumentation for the analysis of total element concentrations as well as complex organic mixtures. As part of contractual research, CAST carries out measurements in cooperation with regional companies such as UniCRE a.s., Spolchemie a.s., Mondi Štětí a.s., Unipetrol RPA, s.r.o. etc.

Ecotoxicology

This laboratory is authorized for the contained use of genetically modified organisms (GMO). Besides equipment for standard exotoxicity testing, it is equipped with a fluorescence microscope, fluorescence microplate reader and a night-shade chamber, which enable work with fluorescent and bioluminescent microorganisms (bioreporters). This enables among other determination of special toxicities such as genotoxicity or endocrine disruption or development of whole-cell biosensors.

Waste Management

The lab-on-wheels (containing mostly mobile facility) enables fast variation of the lab space required for processing larger-scale materials. Waste samples can be cut, grinded, sorted, dried or decomposed for further analyses. It is also about to be equipped with a lab-scale pyrolysis unit, semi-pilot scale photoreactor or GreenGood® thermophile composter. Current research carried out includes recycling of lithium batteries from electric cars, utilization of gastro-waste or photocatalytic treatment of industrial waters.

Laboratory of Remediation

This laboratory is designed for working with contaminated soils, sediments or waters. It is equipped with shakers, centrifuges, 15-litres bioreactor, laboratory-scale photoreactors and calorimeter. Current research includes phytoremediation of contaminated soils, photocatalytic or sorption elimination of pharmaceuticals from waste-waters or preparation of novel sorbents of pollutants from spent materials.

Laboratory of Applied Ecology

The Laboratory of Applied Ecology is primarily used in the practical education of the subjects such as Biology, Ecology, Zoology, Botany and others and also provides technical background for the student bachelor's and master's theses processing as well as the scientific work of academic and scientific workers of the faculty.The laboratory equipment enables the implementation of the ecology studies of the wide range of organisms in the relation to biotic and abiotic environmental factors, including the basic cultivation techniques in microbiology and optical methods.

Laboratory of Soil Science

The Laboratory of Soil Science is used for the practical education and research activities of the students and faculty staff. The laboratory equipment enables the determination of the basic physical and partly also chemical soil properties, such as soil texture, structure, bulk density, moisture, porosity, temperature, determination of the organic matter, active and potential exchange soil reactions, carbonate content, etc. The laboratory also includes the BangCo field laboratory, which enables orientation analyses and fieldwork.

GeoLab

In the geographic information systems lab, also known by the acronym GeoLab, we can find devices for collecting geographic data which serve for the creation of orthophoto maps, 3D models of landscape and buildings, vegetation health analyses and others. One of those devices is, for example, a GNSS device for measuring the exact position. There are also several unmanned aerial vehicles (UAVs) ("drones") available and which can be equipped with variable sensors (multispectral, photogrammetric) for different data collection. 3D printer located in lab is used mainly for 3D landscape models printing.

Laboratory of Photochemistry

The laboratory of Photochemistry focuses on photochemical studies of novel photochemically active compounds, emphasizing the use of photochemistry in solving problems of water environment. The laboratory is equipped with an optical bench set for kinetic analysis, absorption inline fibre optic spectrometer and various photoreactors. For semi-pilot scale studies, UVC photoreactor is available as well.

Laboratory for Synthesis and Environmental Applications of Inorganic (Nano-)Materials

In this laboratory, newly designed and specifically modified conventional "wet" synthetic procedures are used to prepare (mainly) metal-oxide based nanomaterials and composites of low-dimensional (2D) materials (graphene and its analogues). Applications of these materials for environmental protection are examined, for example, as specific or multifunctional sorbents, as so-called reactive sorbents capable to destroy highly toxic chemicals (pesticides, chemical warfare agents), or as materials with antimicrobial or antiviral activities.

2.2 Technische Universität Dresden

Technische Universität Dresden (TUD) is one of the largest technical universities in Germany and one of the leading and most dynamic institutions in the country. With 17 faculties in five Schools, it offers a wide range of 124 degree courses and covers a broad research spectrum. Its focuses Health Sciences, Biomedicine & Bioengineering, Information Technology & Microelectronics, Smart Materials & Structures, Energy, Mobility & Environment as well as Culture & Societal Change are considered exemplary in Germany and throughout Europe. Since 2012, TUD has been one of the "Universities of Excellence". In July 2019, TU Dresden was once again awarded the University of Excellence title and will thus receive permanent funding within the Excellence Strategy of the Federal and State Governments as of 1 November 2019.

2.2.1 Institute of Material Science

The Institute of Materials Science consists of eleven chairs, six of them are cooperative chairs of the TU Dresden with other institutes within the scope of DRESDEN concept and two of them honorary chairs. The institute offers the bachelor degree course and the master course "Material Science". More information is available under: **https://tu-dresden.de/ifww**

2.2.1.1 Chair Biomaterials

The Chair of Biomaterials is part of the Institute of Materials Science, affiliated to the Faculty of Mechanical Sciences and Engineering of the TU Dresden. The main research topics of the chair are biomaterial synthesis for tissue regeneration, biomimetic and bioresponsive materials in contact with cells, as well as their material scientific and biological analysis. Furthermore, surface modification and corrosion processes are investigated. Therefore, the chair is active in various fields, represented in the following research groups.

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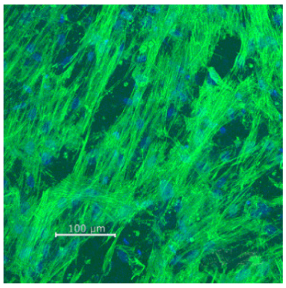
Bioresponsive material systems and bioinspired composites

Head: Dr. Benjamin Kruppke, Benjamin.Kruppke@tu-dresden.de

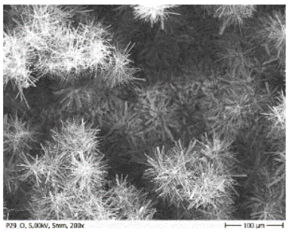
The research group deals with biomimetic mineral formation to synthesise composites for bone replacement. A particular focus is on biomaterial degradation, using the release of biologically active components to stimulate bone regeneration. The focus is on the interaction of bone-building and bone-degrading cells and how this is influenced by biomaterials. Compact materials and porous scaffolds are studied in various projects with respect to their mechanical and biological properties, as well as in special chambers under conditions of fluid flow.



Osteoblasts on organically modified Calcium/ Strontium Phosphate

Corrosion and Surfaces
Head: Dr. Ute Bergmann, Ute.Bergmann@tu-dresden.de

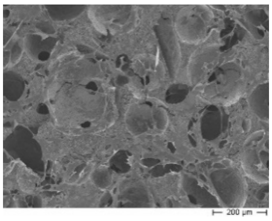
The group deals with the functionalisation of technical surfaces and focuses especially on extensive studies of surficial ice-adherent layers. The team is currently investigating the interaction of ferroelectric coatings with fluid electrolytes. Therefore, the creation of nanostructures by solvothermal methods as well as the physical characterization of the resulting properties by different methods are in the scope of the team. In addition, the group operates a laboratory of electrochemistry and works on corrosion damage cases.



Piezoelectric barium titanate on titanium plates

Functional Biomaterials
Head: PD Dr. Vera Hintze, Vera.Hintze@tu-dresden.de

The research group works on engineering of 2D- and 3D-artificial extracellular matrices (aECM) based on natural biopolymers, like collagen and glycosaminoglycans, including their binding and release of biological mediator proteins. The major focus is on the design of defined, multiparametric cellular microenvironments for tuning cellular responses promoting tissue regeneration in skin and bone and on elucidating the underlying molecular mechanisms. (Bio)materials are analyzed with respect to their mechanical, biochemical and biophysical properties as well the response of skin- and bone related cells.



Human mesenchymal stem cells on aECM-coated scaffolds (REM)

2.2.1.2 Chair Materials Science and Nanotechnology

Research lines:

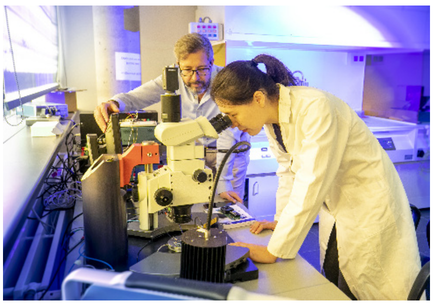
- Nanomaterials for sensor technologies (Dr. Mahdi Samadi Khoshkhoo)
- Computational materials science and theoretical nanophysics (Dr. Robert Biele, PD Dr. Rafael Gutierrez)
- Environmental nanotechnology (Dr. Muhannad Al Aiti)
- Nanoelectronics for sensor technologies (Dr. Bergoi Ibarlucea)
- Machine learning supported digital olfaction (Dr. Robert Biele)
- Tribology of nanomaterials (Prof. Enrico Gnecco)

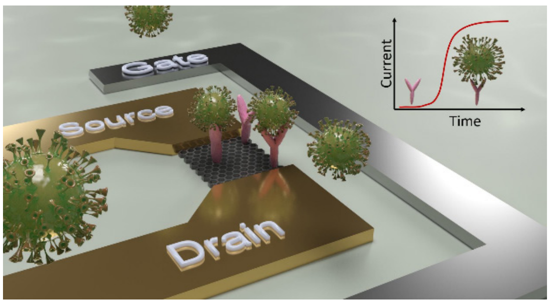
Head of Chair: Prof. Dr. Gianaurelio Cuniberti

complex nano materials

E-mail: gianaurelio.cuniberti@tu-dresden.de
Website: **https://nano.tu-dresden.de**

The research activities of the Chair Materials Science and Nanotechnology focus on the development and integration of novel materials for electronics as well as for energy and environmental technologies. Among other topics, a special emphasis is put on innovative materials for (bio)nanosensors, which are combined with machine learning approaches for signal evaluation to create novel, highly connected and integrated sensor systems. This approach enables flexibly deployable sensor networks, for example for artificial smelling or for the detection of viruses in aerosols (including COVID-19, adaptable to future viral pandemics). Furthermore, our activities deal with materials and principles for energy and environmental technology. This includes the development of battery concepts and materials, the design and prediction of the properties of thermoelectric components, and the development and characterization of supercapacitors, *e.g.* based on nanotubes and graphene. The nanomaterials investigated by the chair also open up new fields of application in wastewater treatment. The topics outlined above go hand in hand with the cross-scale design of nanostructured materials. This includes discovery, development and integration of innovative materials through the use of Big Data and Artificial Intelligence. Newly developed cross-scale and cross-method approaches (ab initio, DFT, Molecular Dynamics, FEM) are applied to digitally describe materials and predict their properties.





2.3 Fraunhofer Institute for Ceramic Technologies and Systems IKTS

2.3.1 Department Bio- and Nanotechnology at IKTS

At the intersection of materials science, biology and materials analysis, the Bio- and Nanotechnology department of Fraunhofer IKTS develops further and optimizes implant materials and their surface properties, developing and using methods of biological material characterization as well as shaping technologies. Beyond the scope of contract research, in-line or stationary test services are also part of the department's portfolio. The researchers work at our locations in Dresden, Leipzig and Berlin and are always in close contact with the client. The aim of our activities is to convert results of fundamental research faster into marketable solutions. This applies to medical equipment in general, as well as to the assessment of the degradation, biocompatibility, and immunological compatibility of implant materials in particular. Nanotechnological approaches for the surface functionalization and additive manufacturing technology play an important role.

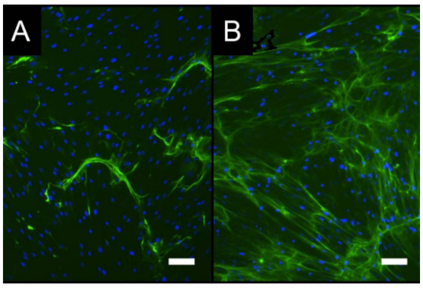
Website: **www.ikts.fraunhofer.de**

Head: Dr. Jörg Opitz, Joerg.Opitz@ikts.fraunhofer.de

Biological Materials Analysis

Head: Dr. Juliane Spohn, Juliane.Spohn@ikts.fraunhofer.de

The development of biocompatible and immunocompatible medical products, such as medical devices and drugs, requires consideration of the interaction between materials or active substances and biology (biomolecules, cells, and tissues) to be able to use them safely on and in humans. The group "Biological Material Analysis" therefore pursues an interdisciplinary approach. At the interface of medical device or drug development and immunobiology, materials, substances and active agents are evaluated, optimized, or newly developed for industrial partners. Standardized diagnostic screening test procedures are also developed for this purpose.

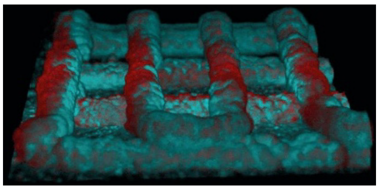


Staining of the generated extracellular matrix by human mesenchymal stem cells (green) without (A) and with inflammatory influence (B). Measuring bar 100 µm.

Characterization Technologies

Head: Dr.-Ing. Malgorzata Kopycinska-Müller, malgorzata.kopycinska-mueller@ikts.fraunhofer.de
Dipl.-Ing. Ralf Schallert, ralf.schallert@ikts.fraunhofer.de

Materials testing and characterization are central components in the manufacture of medical products and medical implants, their certification, and the interaction with biological tissue. The testing of materials and reagents should be gentle, fast, and non-destructive. Ideally, product and method development go hand in hand. The Characterization Technologies workgroup strives to meet this ideal by utilizing, adapting, and developing further established methods of non-destructive testing. These methods include AFM and AFAM, OCT (also combined with additive manufacturing), FFD, µCT, and 3D radiography.

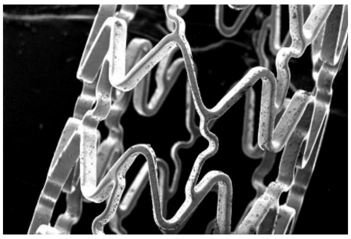


Comparative tomograms of a printed grid-like structure before and after drying; differing areas are shown in red.

Biodegradation and Nanofunctionalization

Head: Dr.-Ing. Natalia Beshchasna, Natalia.Beshchasna@ikts.fraunhofer.de

Tissue and body fluids come into contact with the implant surfaces. The interactions caused by this fact require detailed in-situ monitoring of the various phases of the degradation process. Therefore, the workgroup investigates material changes and aging processes by using synthetic physiological media. Research further focuses on the development of functional nanostructures, as well as wet-chemical thin-film methods, e.g. based on nanodiamonds (sp3 hybridized nanoscale carbon). Furthermore, the group develops approaches for ceramic- and non-ceramic-based biosensors, as well as the corresponding materials and processes for the manufacture and characterization of biosensors.



Accumulation of salts from the simulated body fluid on the stent surface.

Biologized Materials and Structures

Head: Dr. Matthias Ahlhelm, Matthias.Ahlhelm@ikts.fraunhofer.de

Human bones consist of a large number of macro-, meso- and micropores with 100 to 700 µm in diameter. This porosity is especially important for the stability and integration of cells into the bone structure. The researchers produce precise porosities using various replica and placeholder methods or direct foaming techniques. Freeze foaming is one such unique type of direct foaming. It is used to produce potential bone substitute material from materials that are similar to the human body, such as hydroxylapatite or tricalcium powder [$Ca_5(PO_4)_3(OH)$, $Ca_2(PO_4)_3$], allowing the decomposition of the artificial material as the endogenous tissue rebuilds. Bioinert materials such as Al_2O_3 or ZrO_2 may also be used for long-term stable implants. Fraunhofer IKTS evaluates and uses new approaches, such as additive manufacturing, in order to produce patient-specific biomimetic bone structures.

Bone mimicking structure with a 3D-printed covering of dense ceramics and a foam ceramic filling.

2.4 Institute for Complex Materials, Leibniz-IFW Dresden

Website: www.ifw-dresden.de

Leibniz Institute for Solid State and Materials Research Dresden

Institute for Complex Materials
Helmholtzstr. 20
01069 Dresden
Germany

The research activities of the Institute focus on alloy design and processing, chemistry of functional materials and structural analysis.

Chemistry of Functional Materials
Head: Dr. Anne Gebert, A.Gebert@ifw-dresden.de

In the group of A. Gebert, new titanium alloys of the beta-type or metallic glasses are investigated as promising materials to meet the high demands on implants in orthopedics and trauma surgery regarding mechanical and biological compatibility. We analyze relations between composition- and process-conditioned microstructure and morphology and resulting chemical and mechanical properties of those new alloys. In the focus is the materials surface, corrosion and related metal release as well as the generation of tailored surface states are decisive for the optimum interaction with bone tissue and for long implant lifetime. A new research topic is the development of biodegradable Fe-Mn alloys for bioelectronics or stent applications. In addition, owing to their chemical composition and their single-phase nature, beta Ti-Nb alloys are highly corrosion-resistant materials. In body fluids they exhibit extremely low metal release rates, excellent passivity and no indication for local corrosion. This gives rise to a very high biological compatibility. However, alloying additions or second phases can further improve their mechanical biofunctionality or generate antibacterial effects.

Alloy Design and Processing
Contact: Prof. Julia Hufenbach, j.k.hufenbach@ifw-dresden.de

The group of J. Hufenbach focuses beside other topics, on the development of novel biodegradable Fe-based alloys and tailored processes for temporary medical applications. The interest in biodegradable metallic materials for the application as temporary implants has been continuously increasing within the last years. Due to the progressive degradation after providing a temporary support on healing process of a diseased tissue, disadvantages of permanent implants, such as revision surgery, lacking adaption to growth or chronic inflammation, may overcome. Due to the broad adjustable range of mechanical properties, the excellent processability and the high mechanical integrity during degradation FeMn-based alloys are of great interest for (cardio)vascular or urological stent applications. Especially twinning induced plasticity (TWIP) alloys, as e.g. Fe-30Mn-1C-0.25S, are attractive candidates due to their high strength and ductility under tensile load, and moderate corrosion rate, as shown in previous studies. Owing to the excellent mechanical properties, such TWIP alloys show a high potential for the realization of very thin stent structures. Furthermore, in first in vitro cell culture tests a promising biocompatibility was observed.

The aim of these research activities is the development of novel FeMn-based alloys in combination with tailored preparation processes. Hereby, e. g. special casting technologies or selective laser melting (SLM) - as additive manufacturing technique - are applied for tailoring the microstructure and related mechanical, chemical and biological properties.

2.5 TRANS³Net

Website: https://trans3net.webspace.tu-dresden.de/

The border area between Germany, Czech Republic and Poland is characterised by a low level of transnational cooperation between science and industry. Thus, the most important aim of TRANS³Net is to shape conditions for building up a well working innovation system in this tri-national region. This objective will be realised by establishing strong ties and a self-sustaining cooperation between key players of the innovation system and further actors of the scientific, economic and public sphere. By involving all key players relevant for knowledge and technology transfer, TRANS³Net will provide a solution to overcome the multifaceted obstacles concerning transnational cooperation between science and industry.

The network focuses on the continued promotion of transnational knowledge and technology transfer, in particular

- Supporting the successful implementing of knowledge and technology in business
- Supporting the strengthening of companies in the regions by an expedited transfer of usable research results

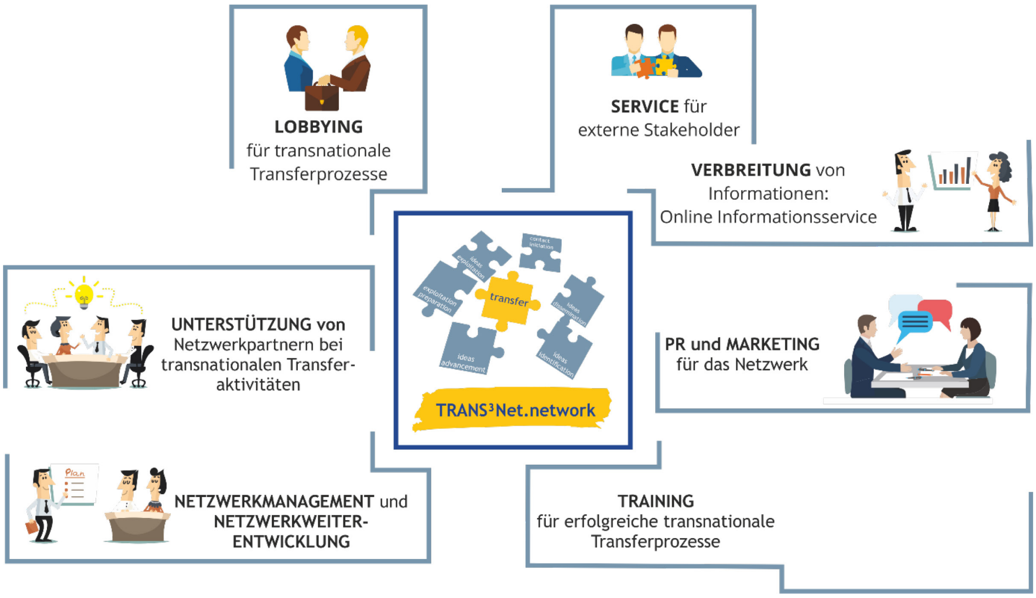
Subject to the availability of funds and the agreement of the partners' authorised representatives, activities will be pursued in the following fields:

- Improvement of cooperation for successful transfer
- Expansion of the information base for effective transfer
- Assistance with the transfer initiation

TRANS³Net plans to achieve its targets in the following ways:

- involving other members in the activities of individual members, e.g. German-Polish Innovation Days, Transferweek, East Saxon Engineering Days, Innovation Exchanges
- jointly organised events and public relations work to support transnational knowledge and technology transfer (esp. TRANS³net.show in the region once a year)
- Using the existing project website (trans3net.eu) to disseminate information about transfer promoters, transfer events, and transfer-relevant funding programmes in the border triangle.
- Providing information and disseminating event announcements etc. via partner-websites.

These activities are organised on a voluntary basis and are planned by individual members or by several members working together, participating in the activities and informing the network about them.



3 Presentation of the PhD topics

3.1 Topic: BIOLOGIZATION

Scientific programme

3.1.1 Exploring the effect of Cu additions on the mechanical behaviour of β-TiNb biomaterials

Ludovico Andrea Alberta

Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Institute for Complex Materials

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Titanium-based alloys are suitable for a broad range of medical applications. Together with 316L stainless steel and Co-Cr alloys, the (α+β) Ti-6Al-4V alloy and commercially pure (CP)-Ti are the most commonly used in the clinical practice for load-bearing implants for orthopaedic applications. However, long-term studies have found out that the large mismatch between the stiffness of the natural bone with that of metallic implant may cause bone resorption and eventual loosening of the medical device. This phenomenon is called "stress shielding" and has serious clinical consequences. For this reason, a new class of low stiffness β-type Ti-based alloys is currently under investigation. These alloys have a single-phase body-centered cubic (bcc) structure which shows lower Young's modulus compared to commercial (α+β) Ti alloys. The use of alloys with reduced elastic modulus have the potential to reduce the stress shielding by improving load distribution to the surrounding bone tissue. Many recently developed β-type Ti-based alloys are based on the Ti – Nb system, which offers a good combination of mechanical and chemical biocompatibility. Recently, we demonstrated that small indium (In) additions up to 5 wt % to Ti-40Nb, which are homogeneously dissolved in the single-β phase, are effective for remarkably decreasing the elastic modulus down to 50 GPa (in compression). [1] Another cause of implant failure, which is raising serious concerns, is biomaterial-associated infections (BAI). These infections are mainly caused by the bacterial biofilm formation on implant surfaces, as a result of the multidrug-resistant bacteria attachment. Bacterial biofilms are highly resistant to conventional antibiotic treatments and therefore it becomes urgent to find new solutions to tackle this form of infection, such as innovative materials with effective antibacterial properties. For titanium-based biomaterials, micro-alloying with bactericidal metals (such as Cu, Ag, Zn, etc) may be a valid option capable of acting against the bacterial colonization of the implant surface. [2]

With the aim of developing new antibacterial Ti-based materials, we have studied a series of ternary TiNbCu alloys obtained by classical metallurgical route (casting + heat treatment). Copper (Cu) is known since ancient times for its antibacterial properties. Various Cu-bearing surfaces and the Cu ions antimicrobial effect have been largely studied by researchers and were shown to be able to act against many bacterial strains, such as S. Aureus and E. Coli with very high sterilization rates (92% and 93%, respectively) [2]. Recently, Cu was used to develop bactericidal ceramics, polymer composites and metallic materials for health care applications. [2]

In the present study we investigated the structure and mechanical behaviour of novel β -type TiNbCu alloys produced by metallurgical route. (Ti-45Nb)-xCu (with x = 2, 4, 6, 8 wt.%) samples in rod shape with 10 mm diameter and ~100 mm length were prepared using a multi-step casting process and subsequent annealing (solution treatment) and water quenching. Solution treatment was carried out at 1273 K for 24 h to dissolve micro-segregations that could form during casting process.

The materials were characterized structurally, morphologically, chemically and mechanically in as cast and heat-treated states. The overall chemical composition of the rods was analysed with inductively coupled plasma - optical emission spectroscopy (ICP-OES). The oxygen and nitrogen contents of the alloys were determined by carrier gas hot extraction (CGHE). Energy dispersive X-ray spectroscopy (EDX) coupled with scanning electron microscopy (SEM) was used to investigate the local elemental distribution. Phase formation and microstructure were investigated and analysed by X-ray diffraction (XRD), complemented by electron backscatter diffraction (EBSD) and SEM. The mechanical properties (Young's modulus, compressive yield strength, elastic energy) were studied by means of ultrasonic non-destructive pulse-echo methods and by means of destructive methods such as static uniaxial compression tests. Vickers microhardness measurements provided additional information about mechanical behaviour of the alloys.

Microstructural examinations show significant difference in the structural morphology of the alloys in the two states. All the as-cast samples exhibit the typical well-developed dendritic morphology. XRD results indicate that when Cu content is below 4 wt.%, a single β-phase (bcc) microstructure is present, while when Cu content exceeds 6 wt.%, a secondary/additional phase is identified, namely the tetragonal compound $CuTi_2$. On the other hand, the heat-treated samples consist of a β (bcc) single phase structure. Solution treatment thus promotes dissolution of the tetragonal compound $CuTi_2$ and ensures chemical homogeneity. SEM results show a microstructure composed of coarse equiaxed bcc-grains with random orientations and a grain size in the range of 400 ÷ 600 μm and a homogeneous distribution of the alloying elements.

Young's modulus is observed to increase with Cu additions, but still remains low (E = 68 ÷ 95 GPa in both states) if compared to Ti-materials in clinical use. Microhardness values ($\mu Hv_{0.1}$ = 184 ÷ 294) show the same trend of the elastic modulus. Static uniaxial compression tests of heat-treated samples show maximum yield strength values (σ_y) in the range of 465 ÷ 604 MPa and a significant Cu-amount-dependent ductility. The alloy with the lowest Cu amount (2 wt.%) displays excellent ductility with no cracking. When Cu content exceeds 4 wt.%, cracking is observed. Their elastic admissible strain (ε) (calculated as $\varepsilon = \sigma_y / E$) is in the range of 0.58 ÷ 0.62, meaning that they can absorb more energy before plastically deforming compared to CP-Ti (ε = 0.46) or SUS 316L (ε = 0.09) [3], thus making them potentially suitable for load-bearing implant applications.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 861046

References:

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3.1.2 Formation of a microenvironment for directed differentiation of stem cells in a perfusion bioreactor

Franziska Alt, Poh Soo Lee, Benjamin Kruppke

TU Dresden, Faculty of Mechanical Science and Engineering, Institute of Materials Science, Chair of Biomaterials,

Franziska.alt@tu-dresden.de

Objective:

Bone is starting from nano-scale, composed of a highly hierarchically organized material, consisting of collagen fibers as organic and hydroxyapatite crystals as inorganic component. Many different cell types are working together in a fragile balance to maintain the bone structure and function. This complex interplay of bone cells and the material components, raise a challenging task, in case a substitute material is needed for bone regeneration. The gold standard for the treatment of large bone defects is autologous bone. Because of its limited availability, decellularized bone is the second choice, providing the natural and wanted composition of organic and inorganic components. In the future, patient-specific artificial bone substitutes may become the new gold standard, owing to their ready availability and the tailored implant design. To ensure the self-healing capability and self-maintaining properties of bone, it is of highly important to mimic the microenvironment of bone cells and to form a stem cell niche, which allows the cells to differentiate into all the needed kinds of bone cells. Therefore, the objective of this PhD project is the fabrication and characterization of 3D-printed polycaprolactone (PCL) scaffolds by fused deposition molding (FDM) that can accommodate a co-culture of different bone cells. The aim of this work is to investigate the microenvironment formed by extrinsic and material inherent properties on the differentiation behavior of human bone marrow-derived mesenchymal stem cells (hMSCs), enabling the production of scaffolds loaded with bone-forming cells in a customized perfusion bioreactor (Figure 1).

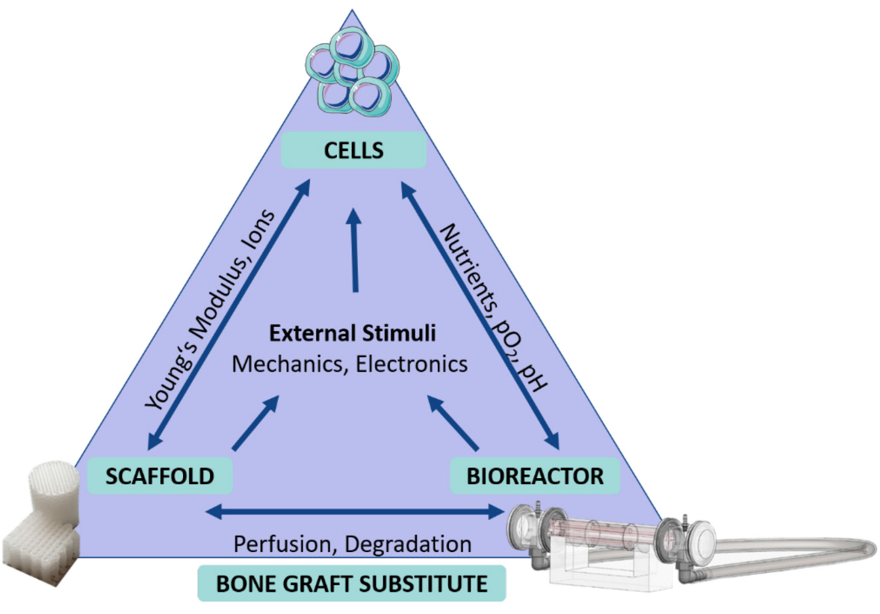

Figure 1: Interplay of perfusion bioreactor, scaffold material and cells to form a microenvironment for bone cells

Procedure:

A perfusion bioreactor has been constructed for cell cultivation in direct contact with the bone substitute material, with the possibility to measure the oxygen partial pressure (pO_2) at various locations, and to exert an electric field (Figure 2). First, the flow parameters and the distribution of an electric field, as well as the distribution of oxygen in the perfusion bioreactor will be simulated, followed by stress-testing with constant measurements of pO_2 and flow behavior in the perfusion bioreactor.

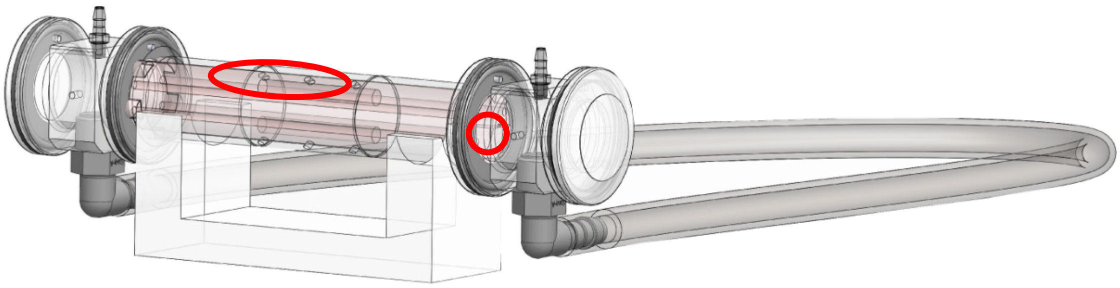

Figure 2: Constructed perfusion bioreactor. The tube in the back is guided through a transformer core to induce transformer-like coupled electrical field stimulation as in [2]. The red circles indicate the holes where partial oxygen tension can be measured.

An important influence on the distribution and concentration of oxygen will be the cell density, which is calculated as oxygen consumption rate per cell in a defined volume. To mimic cell density as present in natural bone, a density of 3 x 106 hMSC per 0,75 cm^3 artificial extracellular matrix (aECM) is targeted. To generate such a relatively high number of cells, hMSCs will be cultured and expanded in spinner flasks. For comparison to conventional cell expansion techniques in 2D, it is necessary to prove the differentiation potential of the hMSC after 3D expansion. For that purpose, hMSC of the same donor were cultured in T175 flasks and on microcarriers with continuous stirring at 80 rpm in spinner flasks, and at the same incubation conditions of 37 °C and 5 % CO2. The hMSC from both expansion conditions were afterwards cultured in osteogenic, chondrogenic and adipogenic differentiation media and stained with Alizarin Red, Alcian Blue and Oil Red respectively.

The PCL Scaffolds will be 3D printed, adjusting the porosity by layer thickness and scaffold architecture. By adding calcium carbonate, the scaffolds shall release biological active ions and furthermore be adapted in terms of their elasticity and wettability to support bone regeneration. Since acidic degradation products are formed when PCL is degraded, the calcium carbonate content must be adjusted so that a sufficient buffering effect can be achieved. Furthermore, the material composition is selected in such a way that the differentiation of the stem cells to bone cells is supported primarily and a degradation rate adapted to the bone regeneration is obtained. For that purpose, degradation tests will be conducted. Finally, the interplay of these three parts – cell density and expansion, physical stimuli, material properties – will be investigated to control the differentiation behavior of hMSCs in a perfusion bioreactor.

Results:

The multipotency of hMSC derived from the spinner flasks was retained and the hMSC could still differentiate into osteogenic, chondrogenic and adipogenic lineages. Furthermore, at least 7 times more hMSC was achieved in a spinner flask than in a T175 flask after 12 days of cell expansion. However, this property is dependent on the applied rotational speed and thus the shear forces acting on the cells. In the perfusion bioreactor, by locally varying cell densities, an oxygen gradient can be achieved, depending on the rate of perfusion. After the design of the bioreactor has been completed with several iteration steps, production is now possible. For the later envisaged application of an electric field for cell stimulation, care must be taken to ensure metal-free production of all liquid-bearing components. Furthermore, the CAD data can be used directly for the flow simulation. Here, first results show the complex conditions during the filling and the continuous perfusion, which require a constructive adaptation of the setup.

In preliminary work using a first generation bioreactor, under hypoxic conditions (< 1 % pO_2), hMSCs preferentially differentiated into chondrocytes, but under normoxic conditions (20 % pO_2), they differentiate into osteoblasts. Thus, both cell types could be achieved in a single scaffold, without the excessive use of biochemical supplements [1].

Several research studies have already shown that the Young's modulus of the scaffold has an influence on the differentiation behavior of hMSC. It is therefore to be expected that the differentiation direction can be locally adjusted by corresponding adaptation of the scaffold geometry, composition or porosity. Thus, it is hypothesized that conditions similar to endochondral ossification can be created in the bioreactor with the support of the variation of the oxygen content [2, 3].

The results from this work will be used to contribute to the study of the influence of physical parameters on hMSC differentiation. By establishing, a well-defined experimental 3D setup that replicates physiological conditions *in vitro*, current limitations of 2D cell culture for tissue engineering can be overcome. With this work, a deepened understanding on the formation of stem cell niches, as well as cell-cell interactions is expected.

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Notes:

3.1.3 Circular microfluidic systems for electro-chemical continuous monitoring of bio-chemicals in emulsion droplets

Dmitry Belyaev

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Droplet microfluidics[1] have shown its effectiveness in a wide range of applications, especially in combination with micro/nanofabricated structures for label-free analysis, *e.g.* amperometric sensors, field-effect transistors, impedimetric sensors and *etc*.[2] Such combination determines a lab on a chip approach for detection of various substances.[3–5] However, the problem of precise droplet manipulation and long-term recirculation over individual sensors still persists. Here we present a microfluidic design that enables such recirculation for the incubation and real-time monitoring of droplets with ultrasensitive nanowire-based impedimetric sensors. The long-term recirculation of droplets over the nanowire area can be used for monitoring bio-chemical reactions whose real-time analysis of the kinetics can be advantageous for a more precise analysis. Aforementioned combination allows long term recirculation of droplets over the sensor which can be used for monitoring of bio-chemical reactions within solutions or cell/bacteria cultures. Generation of hundreds of droplet reactors provides high reliability and throughput of the result due to statistical reasons; precise flow-rate manipulation allows viability of the assay and impedimetric way of monitoring provides immersive analysis of the embedded compounds. Suggested microfluidic design and fluid operation way require precise external syringe or pressure pumps, providing and opportunity to automate the recirculation process. The design of the microfluidic cell fabricated by soft-lithography consisted of an inlets for reactant (water phase), and 3 inlets for oil. Water-in-oil (mineral oil, Sigma-Aldrich, Munich, Germany) emulsion was used. In order to improve the surface interaction and stabilize formed droplets 2% of Span 80 (Sigma-Aldrich, Munich, Germany), surfactant was added to oil solution. The ratio between injection rates of oil and water phases effects the volume of generated droplets and generation frequency. In the presented experiments, the droplet generation frequency was in the range of 1–2 Hz. The injection and guidance of the fluids were controlled with three syringe pumps (neMESYS, Cetoni GmbH, Korbußen, Germany). Fluorinated ethylene-propylene (FEP) capillary tubes (0.8 mm × 0.25 mm, Dolomite, Royston, UK) were plugged in all inlets connected with the syringe to deliver the reactants to the microfluidic chip. We achieved 2-hour recirculation of ~150 water in oil droplets, with the possible detection period of 5 minutes. Further development of described system would require merging of the microfluidics cell with FETs or nano\microwire based sensors. Thus, providing cell or bacteria culture to the water phase (in appropriate buffer) would give an opportunity to continuously monitor the development of ~150 individual cell/bacteria containing reactors.

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3.1.4 Dynamic osteoimmunological crosstalk in a bone replacement context

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In orthopedics and dental applications, each year several millions of implants are being set in patients into and around the bone. A common cause for revision procedures is bad initial healing i.e., new bone formation directly after implantation. The new bone formation and subsequent osseointegration of an implant is a dynamic process that takes place over the course of several months and is divided into three phases: 1) Acute inflammation, 2) Repair phase, 3) Remodeling phase. In the present work, the inflammation phase as well as the initial repair phase was isolated. A prognostic in vitro test scenario for the human new bone formation under inflammatory conditions in preparation for the translation on test material should be established based on previous knowledge from in vivo investigations. The work focused on the investigation of the crosstalk of human mesenchymal stem cells (hMSCs) and proinflammatory macrophages during the selection of physiological culture conditions. The underlying hypothesis of the work was that an in vitro test scenario for the human new bone formation under inflammatory conditions is decisively affected by the combination of hMSCs and macrophages in the processes of immunomodulation and osteogenic differentiation, and that this crosstalk must be characterized before translation onto a material. For this, the THP-1 cell line, a stable macrophage model, was combined with hMSCs from different bone marrow donations. For the development of the test scenario, known physiological events and dynamics from in vivo investigations were applied and cell types were indirectly and directly combined in individual processes to observe the crosstalk and the influences on the processes of immunomodulation and osteogenic differentiation (Figure 1).

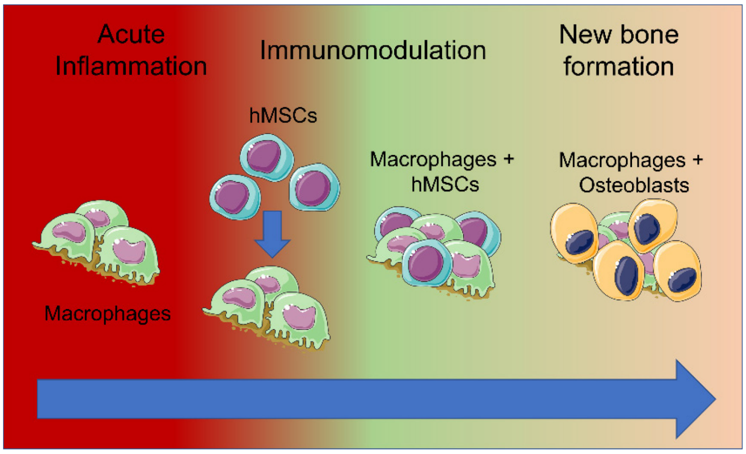

Fig.1 The in vitro test scenario combines the key processes acute inflammation, immunomodulation, and new bone formation after tissue damage in a bone replacement / new implant context. The test scenario combines macrophages, human mesenchymal stem cells (hMSCs) and their interaction as key players in inflammation and new bone formation.

The established test scenario is, through the selected culture conditions, modeled after human physiological processes during and after the placement of an implant and can in the future be translated onto test materials for standardized osteoimmunological evaluation. In comparison to previously published test scenarios, this work considered previous findings concerning new bone formation after implantation and combined these in a model that considered an initial acute inflammation and the resulting immunomodulation. Accordingly, the created test scenario stands out from previously described in vitro test scenarios through the adaption of culture conditions based on the physiologically known processes. Moreover, this test scenario can be utilized for the investigation of active pharmaceutical ingredients. The addition of further cell models or an expansion of the test scenario offers possibilities for the investigation of additional scientific questions, e.g., bone remodeling.

3.1.5 Surface Modification by High-Energy Heavy-Ion Irradiation in Various Crystalline ZnO Facets

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Self-assembled surface nanostructures created by ion irradiation are excellent templates for the deposition of semiconductor quantum dots and manipulation with surface optical transparency. In this work, we have irradiated the surface of c-, m- and a-plane ZnO facets by W ions with the energy of 27 MeV and ion fluences kept in the range $5x10^9$ cm^{-2} - $5x10^{11}$ cm^{-2} to observe the aspects of different irradiation regimes on the surface nanostructuring and optical properties. RBS-C and Raman spectroscopy identify slightly growing Zn-sublattice disorder in the irradiated samples with the progressive damage accumulation for the highest ion fluence. Simultaneously, the strong suppression of main Raman modes and propagation of polar modes indicates high disorder in O-sublattice in the m- and a-plane ZnO. AFM analysis shows the formation of small grains on the ZnO surfaces after irradiation. These nanostructures change optical properties of ZnO crystal and lead to the suppression of NBE and DLE photoluminescence peaks and modify optical n, k coefficients, determined by spectroscopic ellipsometry, exhibiting blurring of particular exciton.

3.1.6 Bioinspired development of artificial enamel via in-situ nano-mineralization

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In recent years, various biomimetic strategies for crystallization and aggregation of apatites have been described. The reproducible replication of biological apatite structures on a microstructural level (3D organized configuration of the crystallites) and thus the intrinsic resistance, still represent a challenge in the context of bioinspired synthesis. In the specific application for manufacturing artificial enamel, nanostructured mineralization is based on the biomimetic formation of hard tissue through an organic matrix and its ordered mineralization with hydroxyapatite crystals. As technical adaption an *in vitro* synthesis is used: a single diffusion step and the so-called double migration method. The processes differ not only in terms of mineral yield, but also in terms of the crystallographic structure of the synthesized, organically modified hydroxyapatite. Both single diffusion and double migration processes exhibit a disordered distribution of the mineral particles, which is why the influences on mineral formation are to be investigated and directed growth should be achieved by adjusting the process parameters. By that way resulting high hardness and abrasion resistance, along with biocompatibility and good degradation properties, are decisive advantages for future potential uses of the mineralization-consolidation approach even beyond the medical field.

3.1.7 Isolation and characterization of plant derived nanovesicles

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Exosomes are small membrane nanovesicles secreted by various organisms, including mammals, plants or fungi. These small membrane nanoparticles can be transfered into nearby or distant cells, and thus they can play an important role in intercellular comunication. For over a decade it has been known that animal cells (including human) produce exosomes, however in plants this ability has only been described in recent years. The presence of exosomes in plants has long been speculated, mainly due to the presence of the cell wall. Today we know that plants secrete structures similar to mammalian exosomes, often called as „plant exosome-like vesicles“. Exosomes mediate cell-to-cell communication by transporting bioactive cargo molecules (proteins, lipids, small RNAs or flavonoids) into target cells, where it can induce changes in gene expression [1–3]. Research has shown that plant exosomes can be involved in plant defense reactions as well as the regulation of symbiotic interactions between plants and other organisms. The findings reveal that plant nanovesicles can also act as biological effectors across species (from plants to animals, including human) where they can modulate various physiological processes. The physiological significance of exosomes is proven by their involvement in disease regulations, such as the formation of cancer metastases or the transmission of pathogenic agents in neurodegenerative diseases [4]. The great attention is paied to the ability of plant exosomes to interact with mammalian cells, as it brings a new possible drug delivery system. Due to ideal native structure and properties, exosomes appear to be a suitable drug delivery vehicles, mainly due to their ability to encapsulate the drug, cross the plasma membrane and deliver the drug into the target site without eliciting an immune response from the recipient organism. The presence of the lipid bilayer prevents the degradation of their contents and contributes to maintaining the stability of the vesicles in cells, thereby reducing the systemic toxicity of the drug. Although mammalian exosomes has the same properties as mentioned above, plant exosomes have a number of specific advantages, wchich make them seem even more suitable for the drug delivery. The most important advantage is the posibility of plant exosomes to naturally carry plant derived molecules. These plant secondary metabolites included in plant exosomes can have various effects

on human health, including antioxidant, antitumor or immunomodulatory effects, that can be transferd together with plant exosomes, providing the additional value to the drug delivery system.
There is number of studies focusing on plant exosomes. However there is no universal isolating protocol. To ensure the optimal results and properties of plant exosomes, it is necessary to select the appropriate method of isolation and to optimizme isolation condition as needed. Here we bring a comparison of isolation methods, as well as the characterization (physical and biochemical) of plant exosomes [5–9].

Key words: plant exosomes, nanovesicles, drug delivery, intercellular comunication

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3.1.8 Dendrimers as Drug Delivery System

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While a conventional approach in cancer therapy brings many side effects, the concept of a targeted drug delivery system (DDS) can open new possibilities in this field. The approach of targeted DDS should be opened by new nanostructures called dendrimers. Carbosilane dendrimers used in our experiments are the new type of nanoparticles with several different modifications, which should be able to fix and deliver the drug to the target tissue.

For evaluation of dendrimers toxicity, the FET test established by OECD with Zebrafish embryos was used. Several different lethal signs was observed over 96 hours each 24 hours by stereo-magnifying glass and inverted microscope. The dendrimers were also conjugated with Cy5 for the observation of biodistribution after microinjection into embryo organism.

The main objective is the determination of appropriate type of dendrimer for other usage in targeted drug delivery in terms of biocompatibility and biodistribution properties. Following the results also the application of dendrimers on xenograft of human cancer tissue cultivated in zebrafish model organism is studied.

3.1.9 Effect of cold plasma treatment of Poppy and Proso Millet seeds in plasma downer

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Every year human population is increasing, thus increasing demands on food and agricultural products. On the other side, adverse environmental conditions, especially water shortage, can lead into reduced germination rate of seeds and then reduced harvest of crops. The plasma treatment is one of the possibilities how to improve it.

A considerable amount of research has been focused on improving the properties of seeds associated with their germination. The aim of these studies was to bring the way how to relieve the stresses connected with soil and ambient environment. [1, 2] Non-thermal plasma treatment can be used as a method of surface decontamination without chemicals, thus interaction of seeds with plasma discharge can sterilize seed coat from attached pathogens. [1, 2] Plasma treatment can change chemical composition of seed surface and change its affinity to water due to surface oxidation. [3] Availability of water is essential for starting of germination process and relieve from abiotic stress. Improved availability of water for seed embryo is not only related to increased affinity to water, but also to erosion of seed coat, thus water transport into seed is easier.[4] Several studies confirmed increased wettability of seeds surface after plasma treatment related to decreased water contact angle. One of the most common ways how to relieve biotic stress is reducing damage caused by pathogens.

The main goal of this study was found optimal conditions of low pressure, non-thermal air plasma discharge treatment in downer type fluidized bed reactor in order to improve poppy and proso millet seeds surface properties and increase their germination properties. Use of plasma downer type reactor is innovative because, unlike previous published studies could offer extremely fast treatment with similar results.

Poppy seeds were put into the dispenser and whole apparatus was evacuated to background pressure about 10 Pa. The ambient air was fed into apparatus to provide required pressure of 100 Pa through the mass flow controller, and then plasma discharge was started in the discharge tube. Power of discharge was varied in range from 10 to 150 W in this study. Seeds were falling down from the dispenser through the valve into discharge tube and then collected in the cyclone separator. The time of plasma treatment of seeds was shorter than 0.1 s. This time was achieved as time of free fall through the plasma zone. The total time of exposure of the seeds to vacuum was shorter than 1 minute.

Despite the very short interaction of poppy seeds with plasma discharge (less than 0.1 s), this time is sufficient for improvement of seeds properties. At the end of germination phase all treated samples had better germination rate than untreated ones. Anyway, only samples modified at 40 W or more had improved germination rate by more than 5 %. All treated samples had significantly increased wettability compared to untreated samples. While untreated samples had water contact angle 85°, all treated samples had contact angles between 19 - 35°. These results can prove connection between wettability of seed surface and their germination rate. With increasing wettability of seeds after the plasma treatment, their germination rate is also increasing. The XPS measurements confirm the wettability results – increased wettability of the treated poppy seeds is related to the higher oxygen content. The deconvolution of the C1s peak also proves, that the most probable functionality responsible for such increase is C=O group. Significant changes are visible in high resolution spectra of C1s peak. The deconvolution of C1s peak shows presence of 3 different carbon bonding groups. The assignment of the groups on the seeds surface was done according to [5] and the positions of the deconvolution components in the software were fixed to chemical shifts given in [5] as well (i.e. 0 eV for C-C group, 1.6 eV for C-O group, 3.0 eV for C=O group).

Seeds of proso millet were treated at the same conditions as poppy seeds. The only difference was power of discharge during treatment. Power varied in range from 40 to 250 W. Effect of plasma treatment on speed of growth and wettability of seeds surface was investigated.

All treated samples had significantly increased speed of growth during first days after planting. The length of root was measured 2 and 3 days after planting. The root length of treated samples was up to 250 % higher than untreated. All treated samples had significantly increased wettability compared to untreated samples. While untreated samples had apparent water contact angle 118°, all treated samples had contact angles between 93 - 101°.

Plasma treatment of seeds in plasma downer reactor brings innovative way for preparation of the seeds before sowing. By setting the right parameters it is possible to achieve improvement in several surface and germination properties.

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3.1.10 Development of new bacteria-killing coatings on beta-Ti-Nb alloy based on functional oxide nanotubular (ONT) layers

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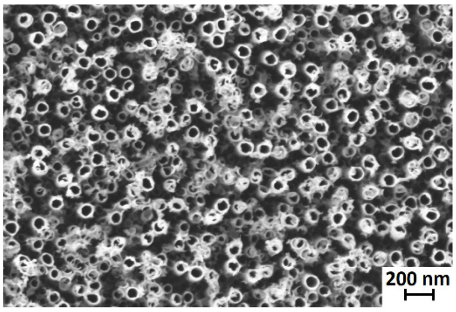
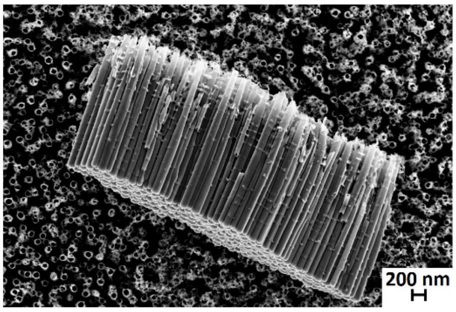
Load-bearing metallic implants should combine the best mechanical functionalities, e.g. low stiffness and high strength, with non-toxicity in relation to low metal release and high corrosion resistance. Beta-type Ti-Nb alloys are therefore promising biomaterials for bone implant applications since they fulfill all these requirements. Specifically, beta-type Ti-(40-45 wt. %)Nb alloys show the lowest Young's modulus values (60-65 GPa (at ST states)) reported so far for binary beta-type alloys. This reveals great potential to reduce stress shielding effects which, in consequence, should minimize risks connected to bone resorption [1].

Surface modifications of such alloys to form porous or nanotubular coatings can further improve osseointegration [2]. Here, Ti-45Nb alloy samples were functionalized with oxide nanotubular (ONT) layers via anodization in an electrolyte mixture of $(NH_4)_2SO_4$ and NH_4F.

To improve crystallinity, samples were annealed at 450°C in air. The obtained coatings were then characterized using SEM, TEM/EDX, XRD, GD-OES, Raman spectroscopy, wettability and corrosion tests. The correlation between the ONT-layer parameters (length, diameter) and synthesis conditions (potential, anodization time) was investigated.



(a)



(b)

Top (a) and side view (b) HR-SEM images of nanotubular oxide layers grown onto Ti45Nb alloy surface

Annealing of TiNb-oxide coatings causes a transition from amorphous to anatase structure; the latter being more preferable for biomedical use. After annealing, an enhanced adhesion between the substrate surface and the nanotubular coating via a barrier-type layer formation was observed by TEM.

A special feature of Ti-45Nb alloy, i.e. the growth of bimodal ONT layer morphologies, was detected. The existence of two pore-diameter size ranges enables designing of a bi-functional coating with improved biocompatibility and bacteria-killing properties. Because beta-type Ti-Nb alloys exhibit limited ability to prevent bacterial infection, additional antibacterial agents need to be supplemented. Conveniently, ONT may also act as containers that can be filled with these agents. Further research will focus on functionalization of these nanotubular layers by metal oxide nanoparticle loadings.

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3.1.11 Algorithms and fluid-dynamic experimental platform for in vitro degradation studies of implant materials

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Based on the 3Rs strategy for animal trials (Replacement, Reduction and Refinement), *in vitro* tests possess an important role in medical device testing. To overcome a still existing gap between *in vitro* and *in vivo* results, replication of the similar physiological conditions in the lab is essentially important. In this work, we present *in vitro* fluid-dynamic experimental setup with in-line monitoring and control of important physiological parameters (temperature, pressure, pH, flow velocity and flow rate) used for degradation studies. Samples of different geometries (square, rectangular and round discs, hollow tubes, polymer films and complex implant structures e.g. stents) can be tested. The setup includes pump, self-designed fluidic chamber providing laminar flow profile, artificial vessels, sensors, circulating waterbath, fluid reservoir, microcontroller unit and a virtual LabVIEW-based instrument with digital and graphical output developed for control and visualization of the parameters. The setup can be used for both short- and long-term experiments and has already been applied for testing of different implant structures. Especially successful studies have been performed on stents consisting of biodegradable and non-biodegradable alloys. Fluidic tests have been supported by the application of various measurement techniques for analyzing the degradation induced changes in implant volume and on the surface.

3.1.12 Interaction of pollutants on nanoceria

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Cerium oxide is a material with many applications, it is important heterogeneous catalysts [1]. CeO_2 nanoparticles can be prepared by various procedures. Modern green chemistry favours low-temperature one-pot syntheses, especially for potential industrial production. Several processes for the preparation of active forms of cerium oxide have been developed at our workplaces. Some of these forms have the ability to decompose highly toxic compounds such as organophosphorus pesticides [2] or even structurally similar neural paralytic chemical warfare agents such as sarine, soman or VX [3].

Synthesis at low temperature was used in this work [4]. Samples have been characterized by physico-chemical methods such as XRD, XPS, DTA, BET, HRTEM and its degradation activity against parathionmethyl was measured by HPLC-DAD. This contribution is focused on interactions of nanoceria with environmentally important pollutant that can be decomposed or at least sorbed on its surface. These substances are usually used as pesticides or medicines. A significant motivation is to help to look for ways to reduce the total amount of hazardous substances in the environment.

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3.1.13 3D spheroid culture for in vitro testing of nanoparticles

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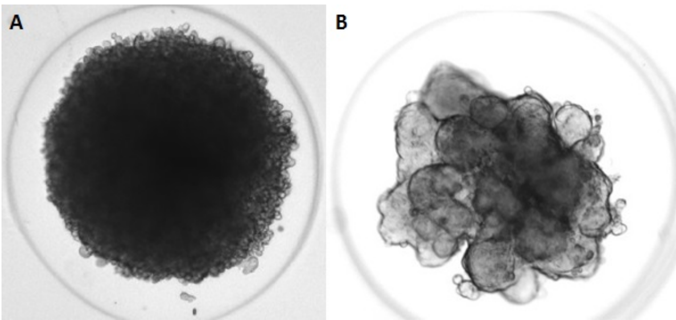
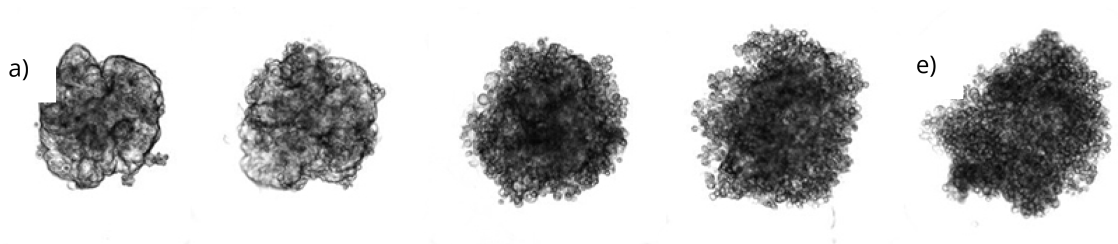
Tumour diseases are one of the most common causes of death in the world. Therefore, it is needed to implement a concept of personalized therapy where an individual patient is subjected to an extensive analysis of the molecular characteristics of tumour cells and tumour sensitivity assays to various available drugs. Most commonly two-dimensional (2D) cell cultures derived from tumour tissue biopsy are used for these assays. However, the response of 2D cell cultures to drugs is different from tumour tissue, which has a much more complex structure. The abnormal cell morphology in 2D culture influences many cellular processes including cell proliferation, differentiation, apoptosis, and gene and protein expression. As a result, 2D-cultured cells may not behave as they would in the body because this model does not adequately mimic the *in vivo* microenvironment. One of the ways to emulate tumour tissue is 3D cell cultures. The effect of drugs observed on 3D cultures is often very different from the effects observed in 2D culture and is very close to the actual effect of the drug on the tumour *in vivo*.



Spheroids cultivated for 96 hours A) Cell line HTB-177 B) Cell line MCF-7

In the first place, open format for 3D cultivation in microarray layout was tested. It is the easiest way for quick, cost-effective testing drugs in a static mode of cultivation. Materials such as glass and biocompatible polymers was modified so that cells cannot adhere, which is the most important condition for spheroid formation. Cultivation of spheroid structures is complicated when their base consists of adhesive flat material. In this case, the surface is covered with a single layer of cells and further growth is inhibited, depending on the signalling pathways. For that reason, 3D Petri dish® technique for spheroid formation was tested. Agarose from 3D Petri dish® was transferred to 24-well microtiter plates and fitted with required volume of tumour cells. During cultivation, growing spheroids were observed by light microscopy. The spheroids was also determinates according to its size and regularity of shape. Growth curves for each cell type (i.e. cell lines) was obtained. Experiments was conducted in order to cultivate tumour cell lines MCF-7 breast, small cell lung adenocarcinoma (cell line CRL-2868) and cell line HTB-177 (large cell lung cancer). Also the effect of nanoparticles and their complexes on the viability and growth of the 3D structures was evaluated. In particular, the cytotoxic effect of nanoparticles was estimated by the growth curves, analysing the ATP production of 3D spheroids with the luminescence method and determining cell viability using the conventional methods (MTT, LDH assays).

The interest of nanoparticles is highly increasing. New possibilities of application move biomedical research on. One type of nanoparticles we are working with is called dendrimers. These are chemical nanostructures, which are interesting because of the good possibility of control of the molecular structure. They offer a possibility of adding desirable functional chemical groups to the periphery of dendrimer molecule. They are able to interact with specifically structures or molecules and eventually to drugs, especially into the target tissue.



MCF-7 Spheroid incubated with dendrimer P(C6H4-OMe)3 at concentration 10 uM; a) Before adding a dendrimer – e) after 96 hours

It is increasingly evident that 3D cell culture models are better models than the traditional 2D monolayer culture due to improved cell-cell interactions, cell–ECM interactions, and cell populations and structures that resemble *in vivo* architecture. There is no doubt that 3D culture systems hold great promise for applications in drug discovery.

3.2 Topic: METROLOGY

Scientific programme

3.2.1 The potential of dendrochemistry and dendroecology in pollution research

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Dendroecology is the science of using tree rings as a proxy to trace changes in the environment [1]. Each ring reflects the growth conditions of a specific time in the past. Annual wood increments can thus provide information on climate and specific ecological processes such as forest fires and insect outbreaks [2]. This can be combined with a dendrochemical analysis, in which chemical variations in tree rings are detected. In the past three decades, research has put forward trees as an archive for environmental pollution. Advantages include that trees are widely available, they can be easily sampled and dated and they provide a high spatial and temporal resolution [3]. However, there are also some limitations. Pollutants are not necessarily kept in the ring of the year they were taken up by the tree, but can be moved via the symplastic or apoplastic pathway. This element translocation is not yet well understood and causes important problems for dendrochemistry [4]. The mobility of chemicals in the xylem depends on tree physiology and structure and the chemico-physical properties of the chemical species [3]. Additionally, the uptake route influences the quantity of pollutants found in tree rings. Trees may take up pollutants from the atmosphere by deposition onto the leaves and/or bark, and from the soil through the roots [5]. Uptake from the soil depends on soil conditions (depth and chemistry) and the structure and depth of the root system [3]. Furthermore, both uptake of pollutants from the environment and translocation within the tree are influenced by climatic variables [6].

The main objective of this doctoral research is to study the potential of using tree rings to map historical pollution. We will evaluate the conditions that need to be fulfilled for dendrochemical proxies to be reliable. One of the factors we will focus on is the thickness of sapwood. Mercury in larch tree rings with relatively thin sapwood has been shown to be a good indicator of past atmospheric Hg concentrations, while this is not the case for Scots pine, a species with a relatively high number of sapwood rings [6]. We will analyse whether the amount of sapwood is an indicator of the suitability of other tree species for dendrochemical analyses. We aim to include diffuse-, ring-and non-porous trees to evaluate whether wood structure influences the outcome. Our study area is Ústí nad Labem, a heavily contaminated environment for which extensive historical air pollution data are available. The sampling of stem cores will be done with an increment borer. We will determine the concentration of different trace metals in the annual rings using both direct (e.g. Itrax Multiscanner) and indirect (e.g. chemical extraction followed by ICP) methods. This will allow assessing the benefits, drawbacks and viability of the different methods for dendrochemistry.

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3.2.2 Development of immobilization protocols for Tro6 and Tro4 aptamers to be used in electrochemical biosensor

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Aptamers are synthetic single stranded DNA/RNA that are developed using the SELEX process to bind to a specific target. The synthesis process of the aptamer allows to introduce modification in the sequence depending on the end application of aptamer. One of the possible applications of aptamers is to use them as receptors as bioreceptors by developing aptamer-based biosensors. Immobilization of aptamers onto the electrode of a biosensor is crucially important for the detection function of the biosensor and its performance parameters.

In our work we introduce the development of immobilization protocols for Tro6 and Tro4 aptamers to be used in electrochemical biosensor for detection of cardiac troponin as a biomarker of multiple diseases e. g. myocardial infarction. To achieve an electrochemical biosensor suitable for commercialization, it is necessary to study the composition and electrochemical properties of the electrode used for the biosensor, to discern a suitable cleaning procedure of the electrode surface before and after biofunctionalization with the bioreceptor as well as to develop an optimal functionalization protocol using an adequate aptamer.

To accomplish this goal this project focus on the aptamers Tro4 and Tro6 developed to bind to the troponin I with a low dissociation constant. These aptamers are commerciality available and have a thiolate 5' end. For the detection of the binding event between the troponin and aptamer we propose to use the redox probes ferro/ferricyanide molecules in a label free approach. Electrochemical measurements such as electrochemical impedance spectroscopy, cyclic voltammetry and differential pulse voltammetry as well as measurements for characterization of sensor electrode surface properties such as contact angle measurements, scanning electron microscopy (SEM) have been employed.

3.2.3 Functionalized electrospun materials for selectvie capture of selected gases

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The global challenge nowadays is the reduction of greenhouse gasses. Our research is focused on the development of polymeric nanofiber membranes prepared by electrospinning for specific functions like selective carbon dioxide and hydrogen capture from waste gas. For this purpose, we follow two research ways: (I.) We are searching for suitable polymers capable to capture selectively CO_2 with a focus on the maximum surface area; and (II.) Searching a polymeric nanofiber carrier for suitable modifiers capable of capturing carbon dioxide. Our membranes for H_2 capture are based on polymer nanofibers based on Pd and Pt nanoparticles. Chemical modification of nanofibers for specific functions is supported by computer design based on molecular modelling, which predicts the stability of nanocomposite composition a consequently the stability of functionality. The crucial role in chemical modification plays the location of modifying agent on the nanofiber surface, which guarantees optimal functionality. This is the key role of technology, which will be presented on some examples of polyurethane and other polymeric based membranes modified by metal nanoparticles.

Keywords: Electrospinning, nanoparticles, gas separation, electrospun polymeric nanomaterials, composite nanomaterials

3.2.4 Applications of gas sensors for air-quality monitoring and identification of volatile organic compounds by GC-HRMS

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Air quality rises major concern since industrial revolution yet we still lack the technology to efficiently keep track of distribution and immision. Network of automated immision monitoring stations provides poor spatial resolution with low scan rate. Copernicus satellite air quality monitoring minimizes these drawbacks but misses the resolution of organic compounds. We can go even further with online on-drone monitoring by sensitive gas sensors for selected parameters and adsorbtion of volatile organic compounds (VOCs) for ex-situ identification and quantification by GC-qTOF instrumentation.

Main part of the work is implementation of suitable commercially available sensors into analytical tool driven by Raspberry Pi, evaluation of sensors performance, determination of best VOCs sampling technique and profiling of these compounds.

Application range for this analytical approach is wide considering extensive atmospheric pollution and significance of various anthropogenic and natural volatile organic compounds. It enables correlation of many parameters linked to spatial distribution, therefore versatile and comprehensive atmospheric research.

Table: Overview of implemented sensors and their essential parameters (excluding supplementary hardware)

Environmental parameter	Operating principle	Operating range	Measurement errors	Scan rate	Resolution	Power consumption
Humidity	Polymer capacitor	5 – 99,9 % Rh	3 % Rh	0,5 Hz	0,1 % Rh	250 μA
Temperature	Semiconducting Si diodes	-40 - 80 °C	0,3 °C	0,5 Hz	0,1 °C	250 μA
Atmospheric pressure	Piezoresistive, temperature compensated	0 – 250 kPa	1 %	Up to 100 Hz **	0.1 kPa	10 mA
Dust and aerosole	Light scattering	0,35 – 12,4 μm	5 %	0,03 – 1 Hz	PM 1; 2,5; 4,25; 10 μm	95 mA
VOC	Photoionization detector (Krypton, 10.6 eV)	1 ppbv to 50 ppmv *	2 %	Up to 100 Hz **	10 ppbv	80 mA
NO2	Electrochemical	10 ppbv – 4 ppmv	2 %	Up to 100 Hz **	10 ppbv	90 mA
SO2	Electrochemical	10 ppbv – 4 ppmv	3 %	Up to 100 Hz **	10 ppbv	90 mA
O3 + NO2	Electrochemical	10 ppbv – 4 ppmv	2 %	Up to 100 Hz **	10 ppbv	90 mA
Air mass flow for sorption tubes	Hot-wire	0 – 2 sdm^3/ min ***	5 %	2 Hz	50 scm^3/min ***	125 mA
Spatial orientation	GNSS	X, Y, Z axes	Signal and environment dependent (~ 3 m)	0,2 Hz	0.00001°	160 mA
* Isobutylene equivalent ** A/D converter setup dependent *** standard cubic centimeter / decimeter (0 °C, 101.325 kPa)						

3.2.5 Prostat, Glioblastoma and Mammary carcinoma cells derived exosomes: Their isolation, characterization and loading with doxorubicin

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Exosomes (EXs) derived from the plasmatic membranes of cells are important indicators of physiological and pathological processes of the organism as well as individual tissues and cells. EXs can occur in various of body fluids and are significant for transport of informatory and regulatory molecules such as protein, lipids microRNAs or they can function as vectors in pathogenesis. Because of that EXs are considered an additional mechanism for intercellular communication and can fundamentally influence the development of metastases in cancer or the progression of degenerative changes, modulation of immune responses. At the same time, EXs are widely studied for their ability to transport embedded regulatory molecules or drugs and can be considered as an alternative to traditional nanoparticle approaches in drug delivery systems. EXs can cross the blood-brain barrier and are therefore interesting transporters for central nervous system (CNS) therapies. The production and composition of EXs depending on therapeutic approaches is still a little studied area that can provide essential information about intercellular communication during therapy. An unknown topic is also the modulation of EXs after interaction with nanomaterials, the transfer of nanomaterials through EXs, and also the possibility of transporting EXs with nanomaterials to the CNS across the blood-brain barrier. Given the widespread field of nanomedicine and the possibilities that nanomaterials offer, such as targeted drug delivery, minimizing the side effects of drugs themselves, or optimizing drug circulation in the body, the transport of nanomaterials via EXs is an important experimental goal [1-3].

Here we present three types of EXs which were isolated from medium of MCF7, PC3 and U87 human cell lines. First, EXs was succesfully isolated using ultracentrifugation. The particle sizes and count of EXs was charaterized by Nanoparticle tracking analysis and Dynamic light scattering. Amount of total and surface protein contain in EXs was measured by BCA assay. Last but not least, protein markers occuring in EXs (CD81, HsP70 etc.) was detected using Western blotting. Second, EXs were loaded with doxorubicin using a simple incubation method. The succes of doxorubicin loading by EXs was measured using High performance liquid chromatography.

The isolation and characterization of EXs from various sources open the potential to future loading of exosomes and their application as natural based nanotherapeutic for the treatment of brain cancer.

Keywords: exosomes, ultracentrifugation, Nanoparticle tracking analysis, Dynamic light scattering, Western blotting, doxorubicin

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3.2.6 Preparation of nanostructured surfaces for CO_2 Detection, Capture and Utilization

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Concerns about global warming have been growing in recent years, the desire for clean energy has risen, less toxic solvents are being used more and more, and in general, humanity is more interested in the environment and its future. There are also growing concerns about rising carbon dioxide concentrations and the consequent greenhouse effect. The technologies currently in use, such as pressure fluctuation adsorption (PSA), cryogenic separation and dry cleaning, still face very high operating costs, high energy consumption and a negative impact on the environment. In contrast, the separation of gases by selective transport across polymer membranes has gradually gained recognition and appears to be a promising candidate for economical and environmentally friendly capture and separation of CO_2. At the same time, it is one of the fastest growing and most promising branches of membrane technology. During the technological development of membrane separation, various strategies have been proposed to resolve the conflict between the permeability and selectivity of commonly available polymeric membranes, with so-called mixed matrix membranes appearing to be the most promising [1,2].

Mixed matrix membranes (MMM) are composite membranes produced by combining an inorganic or inorganic-organic hybrid material in the form of micro- or nanoparticles incorporated into polymer matrix. These membranes can provide separation properties above the so-called Robeson limit, where permeability must be sacrificed for selectivity and vice versa, which is typical for pure polymeric membranes. Various types of inorganic permeable and impermeable materials are used as fillers into MMM. In recent years, the use of nanostructured highly porous materials, such as zeolites or MOF (metal organic frameworks), has become very popular. One of the advantages is that the production of mixed matrix membranes can be adapted to existing polymer membrane production technologies [1-4].

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3.2.7 Chemical modification of PAN – based nanofibrous membranes prepared by electrospinning and their properties for CO_2 capture potential

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PAN-based nanofiber membranes were prepared by a) needleless (wire) = NanospiderTM and b) needle-based electrospinning techniques. These methods differ in the design of the experiment and especially in the form of the electrodes. These differences are further reflected in the structure and morphology, properties of the resulting nanofiber membrane and the dependence of these properties on the parameters that affect electrospinning. Due to the large number of these parameters, process optimization is a necessary part of the work, ie the selection of the most suitable parameters to achieve the desired properties of the nanofiber membrane. Thanks to the large specific surface, nanofiber membranes have the potential to capture a variety of particles and molecules. Their properties, especially sorption, can be further modified and improved by modification, while the modification was performed in a so-called one-step = by adding a modifier to the spinning solution and amines and MOFs (metal organic frameworks) were used as modifiers for CO_2 molecule capture potential.

3.3 Topic: GEOLOGICAL/MATERIALS

Scientific programme

3.3.1 Using biomimicry to design anti-ice surfaces for air-water heat pumps

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The energy transition is one of the most urgent tasks of our time. It can be assumed that heat pump technology will represent a dominant energy supply system in the future. The problem with the efficiency of air-water heat pumps, however, is that they are heavily dependent on external conditions such as the outside temperature and the relative humidity. Frost can already form on the surface of the heat exchanger at temperatures below 3.5°C when the air humidity is above 88% [1]. This frost layer increases power consumption and wastes resources since the heat transfer decreases about 50-75% while the pressure drop increases substantially [2]. The active removal of the ice requires the usage of heat and will lower the COP (coefficient of performance) of the heat pump. Passive coating strategies that either postpone the freezing of covering water droplets or lower the ice adhesion strength would be beneficial in order to save costs and energy [3]. So far, no passive anti-ice solution has made it into a widespread technical application. Using biomimicry might be helpful to choose a strategy that has already proven itself effective in nature. Biomimicry also known as biomimetics uses models or elements of nature for the purpose of solving engineering problems. The objective of this work is on one hand to evaluate the urgency to equip air-water heat pumps with anti-ice surfaces and on the other hand to evaluate how biomimicry might help to rationally design anti-ice surfaces for air-water heat pump applications.

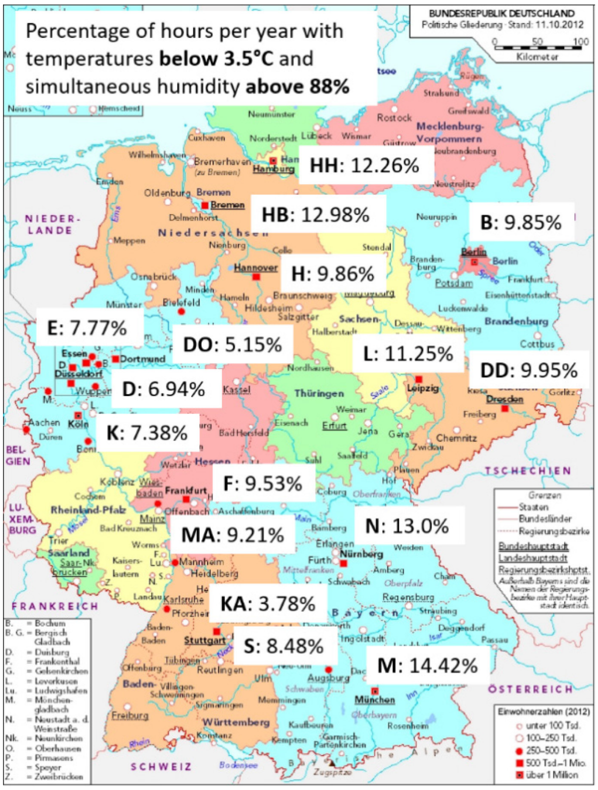

Figure 3: Calculated percentage of hours per year when air-water heat pumps are prone to frost formation and therefore decreased efficiency. CC-BY 4.0 Sabine Apelt

Procedure:

First, a requirement profile for anti-ice surfaces for air-water heat pumps was defined. The urgency to equip them with an anti-ice measures was evaluated by using the hourly weather data for the 16 most populated cities in Germany provided online by Deutscher Wetterdienst (DWD) [4]. A python program was used to count the hours for each station when the temperature is below 3.5°C and the relative humidity simultaneously above 88%. This number was set in ratio to the total amount of hourly data since the beginning of the recording for each station. Then, recent publications dealing with bioinspired anti-ice strategies were collected and sorted. The anti-ice measures found in these papers were evaluated regarding their advantages, disadvantages and applicability for air-water heat pumps.

Results:

Anti-ice surfaces for air-water heat pumps must either substantially postpone the freezing of condensing water droplets or lower the ice adhesion to an extent that naturally occurring forces such as wind or vibrations are sufficient to relieve the frost or ice layerIt is additionally required that the anti-ice surfaces show excellent thermal conductivity, temperature cycling stability between 40°C and -20°C, a high durability in outside conditions for 15 to 20 years with numerous icing and de-icing cycles and resistance against contamination.

Figure 1 shows the percentage of hours for the 16 most populated cities of Germany with temperatures <3.5°C and a relative humidity above 88%. An ice or frost layer might form on air-water heat pumps during these conditions, decreasing the overall efficiency unless additionally power is spend for thermal defrosting. Bio-inspired anti-ice measures might help to lower this additional power usage. The following table (Tab. 1) lists the most widespread bioinspired strategies for anti-ice surfaces found in the literature, their advantages and disadvantages and an evaluation of their suitability for air-water heat pumps.

There are multiple passive anti-ice measures inspired by nature, a more detailed overview of bio-inspired anti-ice strategies is provided by Jiang et al. [15]. However, the technical implementation of bioinspired ant-ice surfaces is usually realized in the form of very complex surface coatings that mostly lack long-term stability and are therefore not suitable for air-water heat pumps, which usually have a service life of 15 to 20 years. Unless natural structures, technical surfaces are not self-healing after the slippery or nanostructured upper layers that provide the anti-ice properties might be deteriorated by contamination, depletion or wear. Another widespread strategy is the removal of incoming liquid water droplets that roll or bounce off the surfaces. This strategy is inapplicable for air-water heat pumps since the heat exchangers freeze due to water condensation and usually not because of incoming liquid droplets. Solar thermal coatings are also not suitable, as their application requires direct exposure to sunlight, which is usually not the case with air-water heat pumps.

Table 1:
Results of the literature review for bioinspired anti-ice surfaces, their advantages, disadvantages and an evaluation of their suitability for air-water heat pumps.

Model Organism & Anti-ice strategy	Advantages	Disadvantages	Suitability for air-water heat pumps
Nepenthes pitcher plant [5, 6]			
Slippery liquid-infused porous surfaces (SLIPS), self-lubricating organogels (SLUG), solid slippery surfaces	+ SLIPS inhibit the accumulation of water and ice through the formation of a chemically-homogeneous lubricating layer, + low ice adhesion, wind or gravity forces sufficient to remove ice layers from surface, + SLUG release oil on the film surface that can be fully returned to the gel matrices by heating the coating above room temperature (self-healing)	~ leakage, degradation or evaporation of the lubricating phase over time ~ increase of ice adhesion and loss of ice resistance due to depletion of the lubricating phase during long-term use	+ very low ice adhesion ~ External forces such as wind needed for ice removal ~ insufficient long-term stability, loss of anti-ice properties
Lotus leaves, butterfly wings, water strider legs [7,8]			
Hierarchically structured superhydrophobic surfaces with contact angles >150° and low contact angle hysteresis, removing of water before freezing occurs and self-propelled jumping of incoming water droplets	+ Removal of liquid water prior to freezing + delay of ice formation caused by decreased heat conductivity of the entrapped air + self-removing of condensed droplets by self-propelled jumping + self-propelling is improved when combined with flexible substrates that vibrate when incoming droplets bounce	~ loss of superhydrophobicity after wear of required nanostructures (repeated icing and de-icing cycles, contamination, ...) ~ potentially transition from Cassie-Baxter to Wenzel wetting state with increasing humidity, decreasing droplet size and temperatures below -15°C that drastically increases ice adhesion caused by interlocking of the ice with the structured surface ~ hierarchically structured surfaces eventually provide more nucleation sites that promote ice nucleation ~ production of nanostructures is costly and difficult to up-scale	+ improved water removal ~ low heat transfer efficiency due to trapped air in the micro- and nanostructures ~ possible failure in low temperatures and high humidity due to wetting state transition ~ insufficient long-term stability, loss of superhydrophobic and anti-ice properties
Echeveria plant [9]			
Asymmetric surface with wavy curvature varying in the micro- and millimeter-range	+ water droplets bounce off + decrease freezing probability due to reduced contact time of incoming liquid droplets + no nanostructures required	~ loss of anti-ice properties as soon as first ice layer is formed and incoming droplets do not bounce off anymore ~ only suitable for precipitating water droplets (e.g. freezing rain)	~ air-water heat pumps do not freeze due to incoming liquid droplets but via water condensation
Arctic fish e.g. winter flounder [10, 11]			
Cryoprotectant-modified surfaces (natural anti-freeze proteins (AFP), AFP mimics such as glycerine, ionic salts, supercharged polypeptides, glucose, urea, deep eutectic solvents, amino acids, choline derivates...)	+ cryoprotectants effectively inhibit ice nucleation by lowering the ice nucleation temperature or increase the freezing delay + polypeptides as AFP mimics are structurally adjustable, non-toxic and biodegradable	~ requires stable mechanical or chemical anchoring of the crypoprotectants on the surfaces ~ some AFP mimics might be toxic ~ some AFP mimics such as amino acids, glucose and others are water soluble ~ low long-term stability of the anchored layer ~ high cost of the extraction of natural anti-freeze proteins	+ effective inhibition of ice nucleation ~ insufficient long-term stability of the anchoring and cryoprotectants

Wheat leaves, ice bear skin [12, 13]			
Solar anti-ice surfaces/ photo-thermal materials, usually combined with superhydrophpbic properties	+ surface temperatures remain above 0°C even under ambient conditions of -50°C and extremely high humidity + melting of accumulated ice through absorbance of incident sun light, anti-reflective and photothermal properties + possible combination with phase change materials that store energy in the daytime and releases heat at cold nights	~ requires sun-light exposure ~ possible structural failure of micro-/nano-porous photo-thermal membranes ~ low long-term stability of the superhydrophobic surfaces (see above) that are required to remove the molten ice	+ higher surface temperatures of heat exchanger might increase efficiency of air-water heat pumps ~ the plates of the heat exchanger are usually not exposed to direct sunlight, even during the day ~ low durability
Antarctic scallop [14]			
Directed ice growth by hierarchical micro-ridges with nanostructures in between	+ ice growth is concentrated on micro-ridges, the regions in between stay ice-free + optimized to minimize underwater ice growth + low number of anchoring points, low ice adhesion	~ requires additional forces such as ocean currents or scallop movement to remove the ice ~ possible interlocking of the ice in hierarchical structures when icing conditions change ~ long-term mechanical stability of the micro- and nano-ridges	+ low ice adhesion ~ external forces required to remove the ice layer ~ insufficient long-term stability, loss of anti-ice properties

Conclusion:

Up to 15% of the year, climatic conditions prevail in Germany where icing up of air-water heat pumps can occur. This usually happens at temperatures when the heat pumps are urgently needed to heat buildings. It is therefore necessary to optimise the defrosting of the heat exchanger and possibly add anti-icing surfaces to achieve the highest possible efficiency (high COP). Up to now, there is no solely passive coating that on the one hand shows low ice adhesion strength and on the other hand a sufficient stability and durability in freezing environments for up to 20 years. It is therefore necessary to investigate possible combinations of the passive coatings with active strategies such as heating or ultrasonic removal of the ice. It is also necessary to standardize the testing methods for the icephobicity of surfaces and to investigate all future anti-icing surfaces for air-water heat pumps in terms of their excellent thermal conductivity and temperature cycling stability between 40°C and -20°C.

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3.3.2 Molecular dynamics of interfacial solution structure of alkali-halide electrolytes at graphens electrodes

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Interactions of graphene electrodes with aqueous solutions of electrolytes play important roles in many technologies such as capacitive deionisation. Particularly important is the surface adsorption of ions due to the electric potential of the electrode. We study structural changes in several prototypical aqueous solutions of electrolytes in contact with graphene induced by its either positive or negative electric charge, at ambient conditions. We carry out molecular dynamics simulations using the most accurate interaction models available. We analyse the solution structure using an advanced analysis of intermolecular bonding, and also standard properties such as density and charge density profiles, electric potential, and screening functions. Our results show that the graphene charge has nearly no translational effect on water molecules, whereas it significantly changes their orientations, and the effect on ion's distributions differ from solution to solution. Larger ions, whose hydration shells are weaker, are affected directly intuitively, i.e., cations are attracted by negatively charged graphene and vice versa, whereas effects on smaller ions may vary and may be even counterintuitive. Regardless of graphene charge, the total number of intermolecular bonds connected with a single water molecule is nearly independent of the distance from the graphene surface and the same applies to the number of intermolecular bonds connected with a single ion, which means that whenever a particle looses an intermolecular bond it nearly always forms a new bond as a compensation.

3.3.3 Metal complexes with polyfluorinated NHCs

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Several transition metal complexes of N-heterocyclic carbene (NHC) ligands bearing polyfluoroalkyl tag were prepared by standard transmetalation proceedure. Precursors [1-methyl-3-(3-(tris(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl) silyl) propyl) imidazolium-iodide] and [1-propyl-3-3(3-(tris(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl) silyl) propyl) imidazolium-iodide] of N-heterocyclic carbenes were prepared by quarternization.[1]

At first all of these metal complexes were characterized by HRMS, EA and multinuclear NMR spectroscopy. Immediately it was apparent that all the complexes were chiral. NHC complexes due to high fluorophilicity do not crystallize, thus Cambridge Structural Database for better understand cause of chirality was used. Was searched for similar structures with deviation of metal-carbene carbon axis from the plane of NHC ring.

These rhodium, ruthenium, and iridum NHC-type organometallic complexes were used in transfer hydrogenation. The standard conditions of catalysis were modified for fluorous biphase system. Observed results of two-phase catalysis and standard transfer hydrogenation were compared.[2,3]

Keywords: N-heterocyclic carbene, Fluorous chemistry, Transfer hydrogenation

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3.3.4 Obtaining of the active mass from the spent Li-Ion batteries

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As the demand for electric vehicles (EV, EVs) rises, rises also the demand for raw materials which are crutial for the production of the Li-Ion batteries (LIBs, LIB), thanks to which are the EVs powered. As the push on recycling is rising, also the prices for the raw materials itself, and the thoughts of independency from the Asian market, the concepts of Gigafactories comes in mind. However the construction of the LIBs can be complicated as it consists from several different parts, metals and elements. Nevertheless the focus on the environment and the protection of the planet should play a higher role in our basic life.

Nowadays, there are several possibilities how the LIBs can be recycled, e.g. pyrometalurgical or hydrometalurgical treatments. There is also a way, which is called as a Direct Recycling (DR). One of the possible DR processes has been described, on the laboratory scale, by *Xiaoping Fan et all* in the article „*Separation and recovery of valuable metals from spent lithium-ion batteries via concentrated sulfuric acid leaching and regeneration of* $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$". Based on the described conditions there have been several experiments made, that proved the possible application in a pilot plant.

Usage of the sulfuric acid (H_2SO_4) for the removal of the polyvinylidene fluoride (PVDF), which is used as a glue that holds the aluminium foil (Al foil) and the active mass (NMC – Ni, Mn, Co) together, is very effective, but only when it comes to high concentration. By low concentration the leaching effect is small and it needs to be supported by manual removal of the active mass. Afterwards has been the hydrogen peroxid (H_2O_2) used, which has several effects: i) separation of the Al foil from the active mass (NMC – Ni, Mn, Co) and flotation effect, ii) reduction effect, which changes the oxidation number of the elements, that is needed for the stepwise precipitation.

Thanks to the ICP-MS analysis, the observation of the experiments and calculating, it can be said that the removal of the PVDF is effective, by the 18M H_2SO_4 roughly 95,4%, by 16M H_2SO_4 90,1%, by 8M H_2SO_4 93,6% and by the 4M H_2SO_4 64,8%. By the lower concentrations, like 8M and 4M H_2SO_4, is the effect low and the PVDF is being removed only partialy and the loosened NMC was supported by manual removal, and therefore these dilutions are not recommended for usage, as there is still a lot of NMC left on the Al foil. Therefore the process, as described in the article, can be applied, but not fully and needs to be modified when wanted to be applied into the pilot plant.

Research highlights:

1) Li-Ion batteries
2) Recycling process – designed recycling
3) Described conditions and their modification – possible application in a pilot plant
4) Usage of the grained materials – recycling as a part of the concept of Gigafactories

3.3.5 Engineering of bio-based Building and Construction Materials

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The global climate change belongs to one of the most critical and important topics of our time. It is mainly induced by carbon dioxide (CO_2) emissions that increased intensively over the last 130 years due to the rapidly advancing industrialization.[1] In this context the cement and concrete production causes about 5-7 percent of the worldwide CO_2 emissions. During the manufacturing process of one ton cement 900 kg CO_2 are released to the atmosphere.[2]

A new innovative method to produce possibly alternative construction materials by engineering living building materials (LBMs) is described by Heveran et al. [3] This technique enables calcite-sand-block fabrication using living organisms. Solidification of the initial materials is induced by MICP (Microbially induced calcium carbonate precipitation). Specific cyanobacteria have shown their potential in a controlled MICP to produce bio-based materials.

Scientific aim of this PhD project is to engineer novel LBMs in a large-scale dimension via controlled CO_2 conversion to calcium carbonate mainly using cyanobacteria. Suitable matrices must be found serving as structural support for the living components and/or as filler materials to fabricate novel LBM constructs with unique mechanical and microstructural properties.

Keywords: Living building materials (LBMs), microbially induced calcium carbonate precipitation (MICP), cyanobacteria

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3.3.6 Degradable bone substitute materials with load-bearing properties - Fiber-strengthened silica aerogels

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Objective:

Highly porous, 3D scaffolds with biomimicking microstructures and load-bearing capacity for bone replacement are still in great demand. In this way, the combination of multiple classes of materials is becoming one of the superb strategies toward the development of biomaterials in tissue engineering applications due to the composite structure of bone. This PhD project aims to develop a novel bone replacement material based on a multi-phase composite system from silica and collagen nanofibers fabricated by electrospinning. At present, a new bi-component electrospinning system is set up and the nanofibers composite is fabricated and subsequently characterized using the Scanning Electron Microscopy (SEM).
The envisioned composites will be formed to a 3D scaffold with material processing (e.g. physical and chemical cross-linking). It is hypothesized that the multidimensional fiber-strengthened composites will provide appropriate mechanical support for a developing tissue and will be capable to properly enhance the cell seeding efficiency, metabolic activity and growth of human mesenchymal stem cells and differentiation to osteoblasts.

Procedure:

To prepare the silica nanofibers, tetraethyl orthosilicate (TEOS) (25, 40, 55 wt %), Ethanol (5 ml), HCl (13 µl), and deionized water (570 µl) was firstly mixed under stirring at 60 °C for 1 h to obtain the silica sol (SiO2). The aqueous solution of polyvinyl alcohol (PVA 7 wt %) was then prepared by stirring at 80 °C. Subsequently, the prepared silica sol was added to the PVA solution and stirred to achieve a homogenized mixture. All chemicals were used as received without further purification. Fig. 1 demonstrates the steps proposed to perform in this project; I) the blend was loaded in a syringe connected to a needle and mounted on a syringe pump. The electrospinning procedure was carried out and SiO2 /PVA nanofibers (NFs) was electrospun. II) In this stage, the nanofibrous composite will be calcined at 800 ºC (muffle furnace) to obtain pure SiO2 nanofibers. III, IV) the silica/collagen (SiO2 /Col) xerogels and aerogels will be produced with the help of SiO2 nanofibers. To this purpose, the electrospun SiO 2 nanofibers will be segmented into small pieces and then uniformly dispersed in fibrillary collagen suspension via a homogenizer and the SiO2 /Col xerogels will be obtained by freeze drying procedure. The obtained short SiO2 nanofibers will be observed by optical microscope and SEM to check the fiber length and distribution. For the preparation of fibrillary collagen suspension, a lyophilized tropocollagen will be dissolved in an aqueous slightly acid solution and then mixed with the neutral phosphate buffer solution to form collagen fibrils (S Heinemann et al., 2013; Sascha Heinemann et al., 2007). Afterward, the SiO2 nanofibers dispersion will be added to the prepared homogenous collagen suspension at various ratios and then vigorously stirred by the addition of a sufficient amount of a crosslinking agent. Finally the freeze-drying procedure will be employed to create a 3D substrate of SiO2 /Col xerogel. Here, we only reported the step for preparing the SiO2 nanofibers.

The flow rate (0.5- 1ml/h), voltage (12- 15 kV), distance between collector and needle tip (12cm) for pure PVA, and the mixture of PVA and TEOS were investigated to obtain smooth, bead-free nanofibers. The morphology of the electrospun nanofibers was also characterized by a scanning electron microscope (SEM).

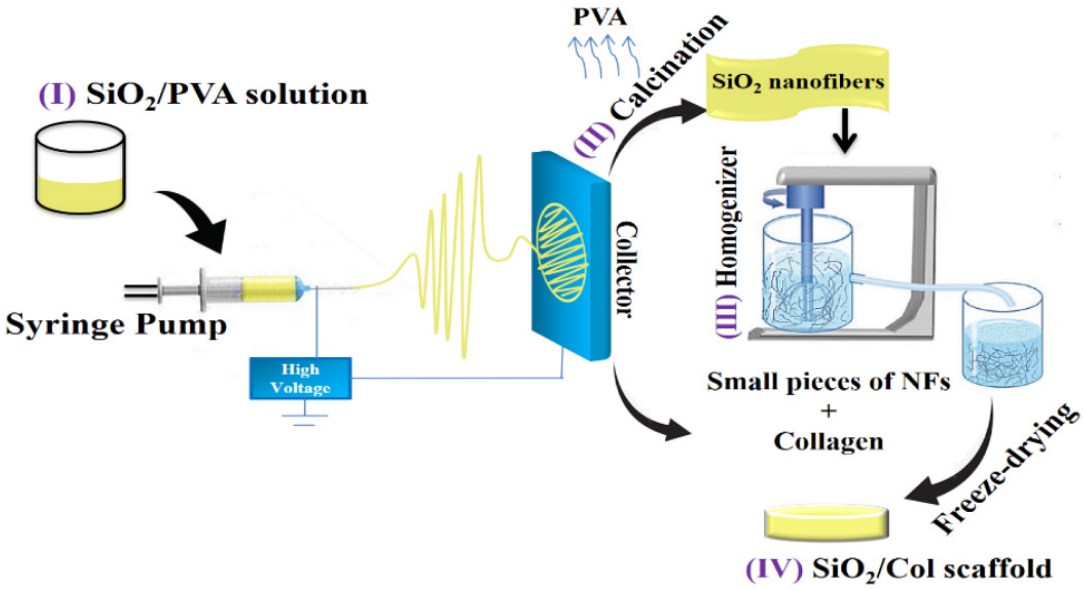

Fig. 1. *Schematic diagram for fabrication of SiO2/Col fibrous composite.*

Results:

Silica with outstanding features such as high mechanical strength and the ability to stimulate both the proliferation and osteogenic differentiation of progenitor cells has received extensive attention in bone tissue engineering. In recent years, several types of research in the Chair of Biomaterials at TU Dresden have been conducted to investigate the role of silica and its composites in bone regeneration. For instance, a composite system, based on the inorganic phase silica and the organic phase collagen at different ratios was developed through a sol-gel process. The results indicated that the incorporation of collagen and silica could positively affect the mechanical properties while the pure silica and merely collagen fibers could not fulfill the mechanical requirements in bone tissue applications (Sascha Heinemann et al., 2007, 2009). Here, as a new approach, our paramount goal is to tailor promising a biomimetic composite with prominent mechanical properties and excellent biodegradability, biocompatibility, and bioactivity which are of special concern in tissue engineering applications. In this regard, we assume that the electrospun nanofibers introduced into xerogels/aerogels can enhance the structural stability or serve as an ECM template to provide a suitable microenvironment for cell growth and proliferation. In this stage of this project, the effect of electrospinning parameters on the morphology of the silica nanofibers was investigated to obtain the randomly oriented NFs. Fig. 2 demonstrates the SEM micrographs and size distribution of the samples fabricated after electrospinning from the solutions containing silica precursor at different concentrations of 25, 40 and 55 wt % with PVA (7 wt %). Pure PVA nanofibers showed an average diameter of 83 ± 18 nm while by adding TEOS to the solution, the average diameters increased to133± 43, 166± 52 and 187± 56 nm for PVA-TEOS 25 wt %, PVA-TEOS 40 wt % and PVA-TEOS 55 wt %, respectively. The results indicated that the nanofibers were uniformly distributed and well separated at different TEOS concentrations and probably due to the increased viscosity of silica network in the precursor mixture, the size diameters of samples increased (Pirzada et al., 2012). Some properties of polymer solutions such as concentration, viscosity and surface tension have the major influence on the size of fibers. As viscosity increases, fiber stretching becomes more difficult, and consequently, thick fibers are potentially produced with broader fiber diameter distribution. In this way, the larger fiber diameter as a result of the increase in viscosity of solutions were obtained for PVA/TEOS comparing to pure PVA nanofibers. On further increase of TEOS concentration (above 55 wt %), the solution became too viscous and created a gelation of the silica precursor which was not appropriate to produce electrospun fibers (Geltmeyer et al., 2016). It can be concluded that the PVA-TEOS nanofibers successfully introduced after optimizing the electrospun parameters and concentration of solutions. In the next step, the produced nanofibers will be calcined at 800 °C to remove the PVA from the nanofiberous composite and obtain pure silica nanofibers which is aimed to be used in the biomaterials composite.

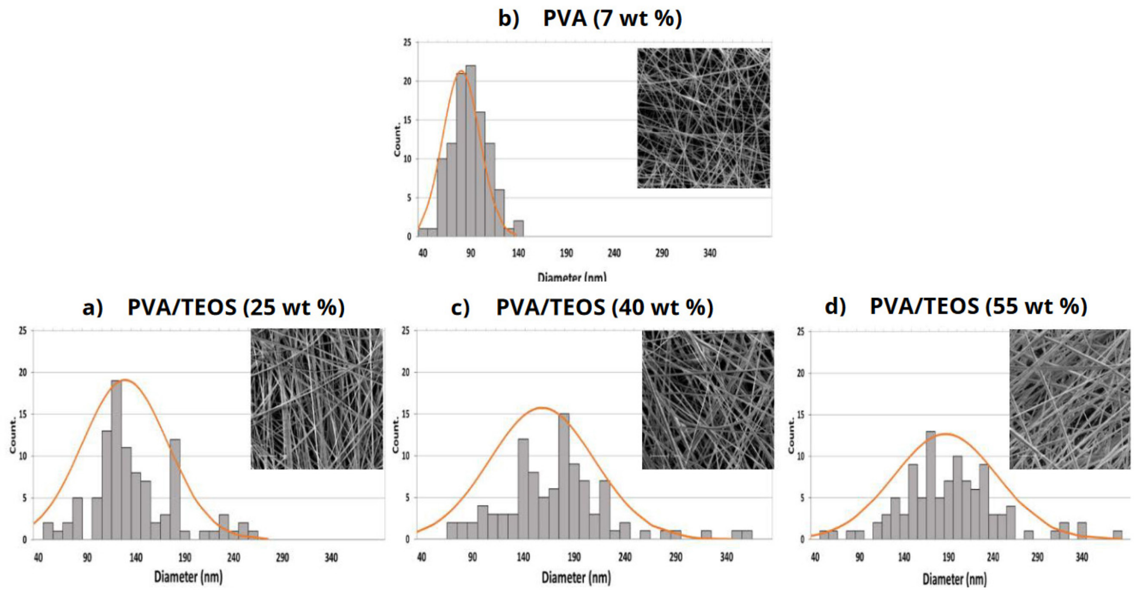

Fig. 2. *SEM images and size distribution of a) pure PVA and b-d) the mixture of PVA and TEOS at different concentrations.*

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Keywords: electrospinning technique, 3D silica/collagen/lignin scaffolds, mechanical properties, bone graft substitute

3.3.7 Preparation of heteroborane derivatives for thin film deposition by the covalent bond formation

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We are engaged in modification of textile fibers and inorganic materials of chemically and physically unusually stable 3D cluster heteroborane complexes with a number of unique properties. Such materials can be used as superacidic heterogeneous catalysts, for selective extraction of cations or some organic matter from solutions, or as special antimicrobial surfaces. [1-3] Our main aim is to prepare starting compounds - heteroboranes with reactive groups and to characterize them by NMR, HPLC, MS methods. We are also testing the catalytic efficacy of new materials in our laboratory. New surface modified materials with a covalently bonded functional heteroboranes are prepared during the chemical reaction in various solvents. Surface modified samples are then tested and inovated in cooperation with other partners.

Keywords: heteroborane – textile – heterogenous catalyst – antimicrobial surface

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3.3.8 The effect of primary and secondary flows on the homogenization process in a vertical bladed mixer

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This contribution is focused on the homogenization process of the dry granular material in a cylindrical mixing device. Although granular flow has been intensively studied, insufficient attention has been paid to the interpretation of the underlying homogenization mechanisms describing the coupling between system dynamics and the local spatial orientation of concentration patterns during the mixing process. Therefore, the motivation is to analyze the homogenization process on the examined system to fill this gap. The results presented here are built on the research previously published [1-4].

The numerical setup was simulated in a vertical cylindrical mixer with two opposed flat blades with a 45° rake angle. The mixing process was performed for 42212 monodisperse colored glass beads of density 2600 kg.m^{-3} with 2 mm diameter and three limit initial packing configurations: tangential (side-by-side), axial (bottom-up), and radial (inside-outside). The development of the homogenization process was examined for the 37 blades' stirrer speeds in the range from 1.9 to 960 rpm. The value of the coefficient of friction was set to 0.1 and the coefficient of restitution was 0.5. Each of the simulated processes was performed for 80 stirrer revolutions. The simulation was conducted using open-source code LIGGGHTS with implemented Discrete Element Method (DEM). The data postprocessing was performed in MATLAB. The development of the concentration patterns, the evolution of the phase interphase and the recirculation zones (introduced and developed by Havlica et al. [1]) were examined. The expansion of the phase interface surface between the particles of different types was used to determine the degree of homogenization as a mixing index. The comparison of all homogenization curves was made by a new integral characteristic, which evaluates the homogenization process using the integral mean value theorem.

Based on the velocities of individual particles in cylindrical coordinates, primary and secondary particle flows were identified. The tangential motion of particles forms the basis of the granular material's primary movement. Because the stirrer's inclination angle is 45 °, the axial movement belongs both by primary and secondary flows. The radial motion of the particles is the least pronounced motion of the particles, which forms the basis of the secondary flows. Generally, these secondary flows are superimposed on the 3D structures of the primary flows. Their presence is not obvious. To observe them, it is necessary to eliminate the dominant primary flows from the raw data. These secondary flows arise from two competing mechanisms: (i) different contact times of particles with the blade (CTM); (ii) different magnitudes of inertial forces acting on particles around the stirrer blade (IFM). At low values of blade rotation speeds, the CTM effect is the primary mechanism, and at higher values, the IFM effect dominates. Each of these mechanisms causes the opposite rotation of the secondary flows. The tangential configuration is best mixed due to the possibility of immediate engagement of primary flows with high kinetic energy into the homogenization process and due to the spatial non-uniformity of this flow. Radial and axial configurations generally have a slower start of the homogenization process due to the need to involve mainly secondary flows in the mixing process. An exception is blades' rotational speeds, where a large radial macroscopic flow of particles is created behind the agitator blades due to the centrifugal force. This phenomenon causes considerable expansion of the phase interface and allows almost immediate involvement of the primary flows into the mixing process. For these blades' rotational speeds, the homogenization process is almost independent of the initial packing configuration. According to these findings, three basic rules were identified to achieve effective homogenization. These rules determine the synergy between the phase interface and the particles' motion.

3.3.9 Molecular Simulation of Salt Hydrates

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Salts are among the most important substances on Earth. Simulation studies of salts in aqueous solutions and anhydrous crystals are now common. However, almost nothing can be found in the literature regarding molecular simulations of salt hydrates. Their first successful molecular simulations have appeared in the literature only recently, and only in the case of hydrohalite, or sodium chloride dihydrate ($NaCl \cdot 2H_2O$). Since hydrohalite crystallizes in a monoclinic system, simulations of its modern polarizable models alone are difficult to realize. It is not surprising, therefore, that results for the properties of crystal hydrates obtained from molecular simulations cannot be found in the literature, nor a description of the relevant methodology required. The properties mentioned are the values of lattice constants and atomic deflection parameters.

This master thesis deals with the determination of properties of salt hydrates from molecular simulations. We focus on developing a methodology for determining crystal lattice parameters and atomic displacements from molecular simulations using polarizable ion models, which is applied to a hydrohalite crystal. The methodology involves the application of specific boundary and initial conditions.

The results are compared with experimental data from the literature. The resulting lattice parameters are in good agreement with experiment, and the atomic displacement parameters are also in reasonable agreement, although some results underestimate the experimental values, which can be attributed to inaccuracies in the interparticle interaction model, effects of the finite size of the simulated crystal, or inaccuracies in the experimental data and ambiguities in their precise meaning.

3.3.10 Surface functionalization of Ti_3C_2T MXene for MRI contrast agent

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MXenes are a unique class of two-dimensional metal carbides and/or nitrides that have shown great potential for many purposes, e. g. for medical applications, especially diagnostic approaches. The main aim of this work was to enhance the magnetic properties and response of the Ti_3C_2T MXene flakes for bioimaging. Because of the diamagnetic nature, MXene flakes were grafted with chelating agent diethylenetriamine pentaacetic acid in order to entrap Gd^{3+} ions. This strategy of functionalization caused transition from dia- to paramagnetic properties of MXene flakes. Also, dependence of magnetic relaxation time on flakes concentration was observed. This fact made it possible to estimate the spatially differentiated distribution of MXene flakes. Chelation of Gd^{3+} ions also prevents leaking compared to electrostatic interaction. Moreover, surface was protected against oxidation and agglomeration in phosphate buffer saline and blood serum. Additionally, mammalian cell-based tests were also performed and indicate the low level of material toxicity, suitable for medical applications. All stages of the surface modification were confirmed by several analytical techniques, suggesting the changing of flakes surface termination, surface properties, including the retention of the plasmon absorption band, required for photothermal application. Paramagnetic MXene-Gd flakes were subsequently demonstrated to be a good T_1 contrast agent for MRI with the ability to the time-resolved estimation of flakes distribution and local concentration. The created material can be used for contrast MRI and photothermal treatment with a higher degree of stability and cytocompatibility. Potentially, the created material can be subsequently used for theranostics applications, where the imaging can be combined with phototherapy [1].

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3.3.11 Fuel characteristics of Miscanthus x giganteus biomass produced at the marginal and slightly contaminated by trace elements soils

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Miscanthus x giganteus has been identified to successfully remediate sites slightly contaminated by TEs, or marginal lands with production of biomass for bio products or energy. The use of *M.xgiganteus* biomass as an alternative energy source positively contributes to climate change mitigation. The aim of this study was to analyze the properties of *M.xgiganteus* biomass in thermochemical transformation by gasification and how the process may be impacted by conditions of the background production of the crop. Varied combustion properties of Mxg from different locations and plantation types were investigated. The input materials from two plantations in Ukraine (marginal-Tokarivka) and contaminated (NULES, Kyiv), Croatia (agricultural), and Czech Republic (post military-Chomutov) were evaluated. The proximate analysis (determination of ash content, total water, volatile matter), calorific value and ultimate analysis (content of C, H, N and S) were done based on German and international standards (DIN and DIN ISO). The ash melting behavior and temperatures of samples was analyzed using a heating microscope as criteria of biomass combustion quality. Low ash melting temperature can lead to slagging of the process and thus to serious technical problems during gasification. Results showed that ash content and volatile matter of the various *M.xgiganteus* are significantly different based on location with an average of 4.9% and 78.1% respectively. The calorific value of the different biomasses was high, ranging from 18 to 19 MJ/Kg. The highest calorific value was received for *M.xgiganteus* produced in Kyiv despite Pb contamination in soil. The average final melting temperature of *M.xgiganteus* was 1323 °C, a medium meltable ash, suitable for gasification.

Key words: *Miscanthus x giganteus*, bioenergy, gasification, ash melting temperature

3.3.12 Bioresorbable Fe-based alloys processed via laser powder bed fusion

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Aiming for the fabrication of patient-specific implants, a strong research focus is set on additive manufacturing (AM) techniques. Because of their high freedom of design, they open up new possibilities for load-adapted implants. This is possible due to the additive, layer-wise manufacturing, which also enables function integration into the implant design [1,2]. Especially laser powder bed fusion (LPBF; also known as selective laser melting, SLM) shows a large potential for the fabrication of both, customized and filigree metallic implants.

The LPBF process enables high cooling rates through local melting. Therefore, specific non-equilibrium microstructural effects can be realized, e.g., grain refinement, extended solid solubility and the reduction of the fraction and size of segregated equilibrium phases. Such effects can be very beneficial for the resulting mechanical and chemical properties. Additionally, the manufacturing of near net-shape filigree structures can be achieved thanks to a small powder particle size and a fine focused laser beam. Thus, LPBF offers a great potential for the manufacturing of load-adapted implants with tailored microstructures. Nevertheless, in close vicinity of the laser melt track, which is surrounded by non-molten metallic powder particles and underlying solidified bulk material, the large temperature gradient results in a rather directional solidification. This may lead to elongated grains and crystallographic anisotropy, respectively defined as texture. Together with specific defects of the layer-by-layer manufacturing such as inclusions, porosity and residual stress, this may result in multi-scale microstructural anisotropy. By process control, e.g., with adapted scan strategies or the application of a substrate plate heating, the microstructure can be tailored for different grain morphologies, textures and phase compositions while reducing the defect formation at the same time [3]. Nevertheless, the LPBF anisotropic material behavior has to be considered or can be exploited for potential implant applications.

For medical device applications LPBF has been intensively used for several non-degradable, metallic biomaterials, such as Ti-based or CoCr-based alloys, AISI 316 L steel as well as noble metals, shape memory alloys or bulk metallic glasses [4–9]. In contrast, bioresorbable metallic materials based on magnesium-, iron- and zinc are particularly advantageous for temporary implants, but their processing, via LPBF, especially for Zn- and Mg-based systems, is only investigated in an early stage, yet [4,10,11]. Nethertheless, the intention for processing biodegradable metal materials via LPBF for, e.g., stents would be the advantage of a patient specific design combined with a mechanical and healing support for the damaged tissue and full implant resorption after completing the task. Therefore, they overcome challenges like revision surgery, chronic inflammation or lacking adaptation to growth when the implant is deployed at infancy. Mg-alloy based implants processed by non-AM technologies are already commercially available. The drawbacks of Mg-based materials are an excessively fast degradation and adverse hydrogen gas evolution for some applications [12]. Additionally, their low mechanical strength does not allow their use for thin strut and therefore low weight vascular stents. In contrast, iron-based alloys are a promising alternative to magnesium alloys since they offer the high mechanical strength, ductility combined with a good processability, also by LPBF. Iron is an essential element in the human body, e.g. it is involved in oxygen transport and functions as a component of metalloproteins. It is therefore considered as one of the most biocompatible elements [13]. A challenge of iron-based alloys is their slow in-vivo corrosion rate, which is mainly caused by the formation of degradation-inhibiting orrosion product layers. Enhancing the corrosion rate can be achieved by alloying (e.g. with Mn, Pd, S), coatings or applying special manufacturing technologies [14–17].

In this doctoral thesis new resorbable Fe-based materials for LPBF-processing of stent implants are developed. The focus lies on manganese steels due to their proven suitability for LPBF, adjustable strength and ductility, high integrity during degradation over several months and adequate biocompatibility which makes them promising for stent applications [18,19]. The new materials have to exhibit enhanced mechanical and corrosion properties in comparison to the promising, bioresorbable Fe-30Mn-1C-0.02S alloy [20] and the clinically applied AISI316 L [21,22] as reference materials. A sufficient biocompatibility and ideally an incorporated antibacterial effect are additionally necessary properties. For the microstructural characterization scanning electron microscopy (SEM) coupled with energy dispersive X-ray spectroscopy (EDX) and electron backscatter diffraction (EBSD) are used. The mechanical properties are investigated by Vickers hardness testing and quasi-static compression and tensile measurements. For the degradation evaluation potentiodynamic polarization (PDP) and immersion testing in simulated body fluids (SBF) are used in combination with degradation species analysis techniques such as fourier-transform infrared spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS). For promising alloy variants, the investigations should be supported by cell viability and antibacterial studies. Thus, as a result the combination of both, additive manufacturing and bioresorbable FeMnC-based alloys may lead to innovative patient life-saving implant.

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3.3.13 A millifluidic chip for cultivation of fish embryos and toxicity testing fabricated by 3D printing technology

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Zebrafish (Danio rerio) have become a very popular animal model. Their embryos have been widely used in acute toxicity tests, the so-called fish embryo tests (FETs). Over the last years there has been an effort to develop various systems for a high-throughput zebrafish embryo cultivation and FET testing. In this work, we present a novel design of a microfluidic system fabricated by 3D printing technology and we evaluate its functional properties for zebrafish embryos cultivation and toxicity testing.

The development and the optimization of the microfluidic chip was performed by CAD (computer-aided design) modelling, based on CFD (computational fluid dynamics) simulations and real experiments. The embryos are trapped inside the system by free sedimentation by gravity. An equal flow around the embryos through two separated channels has been achieved with a single water inlet. This ensures sufficient medium exchange and prevents accumulation of substances on the bottom of the cultivation wells.

An individual embryo removal functionality, which can be used during the cultivation experiments for selective unloading of any of the cultivated embryos out of the chip, was added to the chip design. This system consisted of narrow lateral channels leading to the bottom of the well of each embryo. When a flow pulse was applied to the selected lateral channel, it resulted into lifting the embryo up and flushing it away trough the upper flow channel. This unique property raises the possibility of detailed studies of the selected embryos by additional methods. However, it requires complex tubing (24 for each chip) with a reliable flow switch and the experimental execution of this system still poses a challenge, especially with more chips used simultaneously.

The chips were manufactured by DLP (digital light processing) 3D printer. This method allowed easy fabrication directly from the CAD and has proven the capability of printing complex inner channels with sufficient resolution for our purposes. The limited transparency of the used material was solved by fabrication of the device as a two-component system with a transparent foil laminated to the bottom part of the chip.

Long-term cultivation experiments have shown a normal development of zebrafish embryos in the chip, when the freshly 3D printed material was leached in ethanol prior to use. Model toxicity tests were further performed with diluted ethanol as a teratogen. Compared to the FET assays, an increased toxic effect of the ethanol on the embryos cultivated in the chip was observed.

We conclude that the presented 3D printed chip is suitable for long-term zebrafish embryos cultivations and toxicity testing and we have plans for future development leading towards more compact and more convenient system for automated FET assays.

Keywords: Zebrafish, FET, 3D printing, microfluidic, millifluidic

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3.3.14 Unlocking mass production of photocrosslinked chitosan nanofibers

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Chitosan nanofibers are a promising material for a wide range of biomedical and filtration applications thanks to unique properties of both the polymer and the nano-form. However, solubility in aqueous solutions limits their performance in these fields and needs to be solved by an additional crosslinking. Developing an effective way of crosslinking during mass production is a crucial step in unlocking the full potential of chitosan nanofibers. Therefore, we have modified chitosan by methyl methacrylate, which allowed fast photocrosslinking of resulting nanofibers by UV irradiation. Crosslinked nanofibrous mats from modified chitosan showed increased resistance to aqueous solutions and had no harmful effects on mammalian cells in cultivation experiments. During the process development, we have cooperated with an industrial partner and it will be used in a scaled-up version thanks to its compatibility with a continuous production line.

3.3.15 Adsorption and Diffusion of Short Hydrocarbons and Carbon Dioxide in Shale Organic Matter: Insights from Molecular Simulations

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In today’s world of rising energy demands there is pressure to find new and unconventional sources of energy – and hydrocarbons extracted from shale rock is one of those resources. Shale consists of two distinct parts: inorganic (mostly clays and quartz crystals) and organic (kerogens, hydrocarbons, asphaltenes and other compounds). This work focuses on organic part of shale, which differs in form and composition depending on its maturity, place of origin and type of organisms decomposed to create the material.

We use different approaches to create microporous organic matter models (mimetic and reconstruction ones) and adding either slits or cylindrical pores to encompass mesoporosity and therefore create dual-porosity organic matters. Those models correspond to organic matter of different types and maturities allowing us to study range of behaviours related to confined fluids. To study hydrocarbons and carbon dioxide we utilize existing models (both united atoms and all atoms) since there is wide existing selection.

The main focus of the work is adsorption and diffusion studies using methods of molecular simulations, namely employing Monte Carlo method to study equilibrium adsorbed amounts (and competitive adsorption when applicable) and molecular dynamics method to study diffusion rates. In general, after creating models, we evaluate chemical potential at studied temperatures and pressures which we later use as an input in Grand Canonical Monte Carlo to calculate equilibrium adsorbed amount. Then, we use the equilibrium amount and a snapshot of molecules positions to start the molecular dynamics simulations to retrieve trajectories which are the foundation to evaluate self-diffusion coefficients and other interesting properties such as density profiles which allow us to glance in the molecular makeup and behaviour.

In general, when studying adsorption of methane and carbon dioxide mixtures (meaning studying competitive adsorption), there is preferential adsorption of carbon dioxide over methane suggesting possibilities of enhanced shale gas extraction and carbon dioxide sequestration. When studying diffusion there is inverse relationship between adsorbed amount and self-diffusion coefficients, meaning that the higher is the adsorbed amount, the lower is the self-diffusion coefficient.

Keywords: adsorption, diffusion, molecular simulations, molecular dynamics, Monte Carlo methods

3.3.16 Investigating the material hardness of mollusks shells in dry and wet states by microindentation

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The fracture behavior of mollusk shells differs markedly from the fracture behavior of calcium carbonate, from which shells are mostly made [1]. Understanding this material behavior and transferring it into modern materials can open new pathways to more durable materials. Therefore, the material behavior of shells is examined in this poster.

The fracture behaviour of shells strongly depends on the orientation of the prismatic layer, shown in Fig. 1 [2]. As depicted in Fig. 2, the structure withstands a higher compressive stress when the load is applied along the prisms (a) compared to when the force is exerted perpendicularly (b). In further experiments two different cracking mechanisms were observed. While loading the structure in the direction of the prisms led to a stopping of the cracks at the organic part, the second case revealed a catastrophic cracking of the specimen through the prisms, as illustrated in Fig. 3.

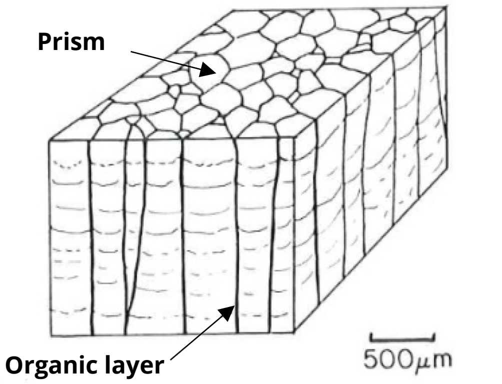

Fig. 1: Schematic representation of the prismatic layer composed of prisms surrounded by organic layers. [3]

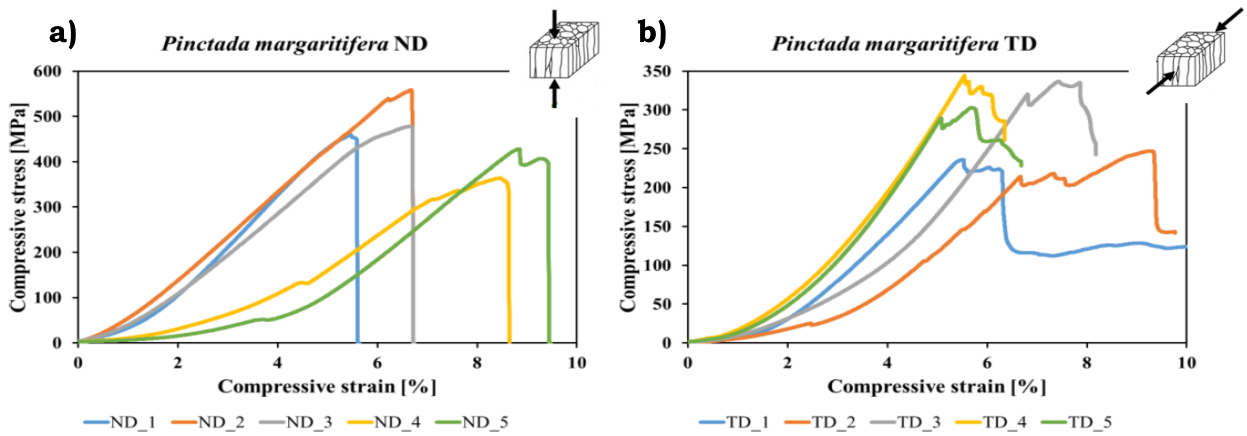

Fig. 2: Strain-stress curves of a P. margaritifera shell for compression tests along the depicted orientation. [2]

In the poster, microindentation tests are employed on P. margaritifera shells to perform the fracture experiments for dry and wet specimen.

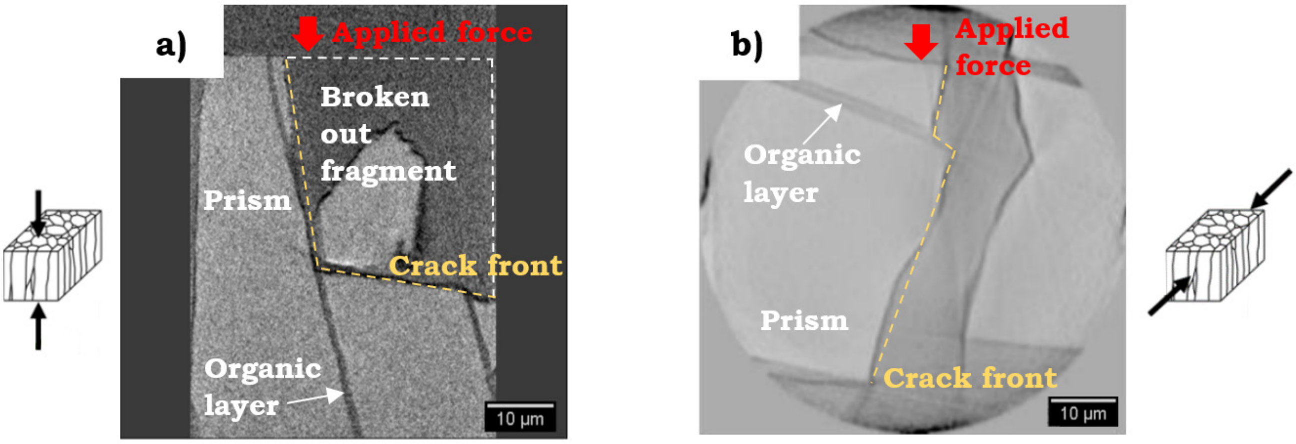

Fig. 3: X-ray images of P. margaritifera shell after microindentation. (a) Crack stopped by the organic layer. (b) Catastrophic failure of the structure [4].

Results

The experiments carried out are consistent with the anisotropic mechanical properties of P. margaritifera shells published by [2]. While the organic layer stopped cracks that grew in the direction of the prisms, crack development was not stopped when it developed perpendicular to the orientation of the prisms. The comparison of wet and dry shells showed no clear differences. In terms of crack growth, the dry and wet experiments revealed similar anisotropic crack growth behavior. Regarding the indentation force for crack initiation, the results do not allow a clear distinction between the required fracture forces. While in the dry experiments the force along the growth direction was 87 mN and in the orthogonal case 95 mN, the force in the wet condition is higher with 175 mN in the perpendicular case than for the indentation along the prisms with 33 mN. Since each experiment was performed only once, the results are not statistically significant. To obtain results with statistical significance, further experiments must be carried out.

Keywords: X-ray imaging, microindentation, mollusk shells, mechanical testing

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