FLOW AND MATERIAL SIMULATION

Together with the Institute for Composite Materials (IVW), we are developing simulation methods for virtualizing sheet molding compounding of fiber-plastic composites at the “High Performance Center for Simulation- and Software-based Innovation”. The picture shows the SMC plant with thermoset impregnation and suction system in the IVW pilot plant.

DR. KONRAD STEINER
HEAD OF DEPARTMENT

MULTISCALE AND MULTIPHYSICS METHODS AND SOFTWARE SOLUTIONS FOR INDUSTRIAL APPLICATION

Our department Flow and Material Simulation develops multiscale methods and software tools for the product development and the corresponding process layout. One of the typical challenges for us is to control the mutual influences of manufacturing processes and the multifunctional, local material properties by means of simulations. The unique of the department lies in the development, enabling and specific use of multiscale and multiphysics methods and customer-specific software solutions suitable for industrial application.

Already by name, the department can be divided into two large fields of competence: "Computer-assisted material design and microstructure simulation", enables to simulate and optimize numerically the functional characteristics dealing with porous materials as well as composite materials. There is a strong demand for our highly efficient, micromechanical methods for the material design of fiber reinforced composites and technical textiles. The "simulation-assisted design of complex flow processes" works on the corresponding manufacturing processes such as mixing, dispersing, injection, filtration, coating and segregation. Focusses of the industrial application are processes of filtration and segregation as well as the product design of filter systems or other process equipment.

The projects of application often address material design as well as flow simulation. Thus in the area of electrochemistry, we are engaging in diverse aspects for the appropriate material of battery cells or fuel cells as well as in their production, e.g. the filling of battery cells.

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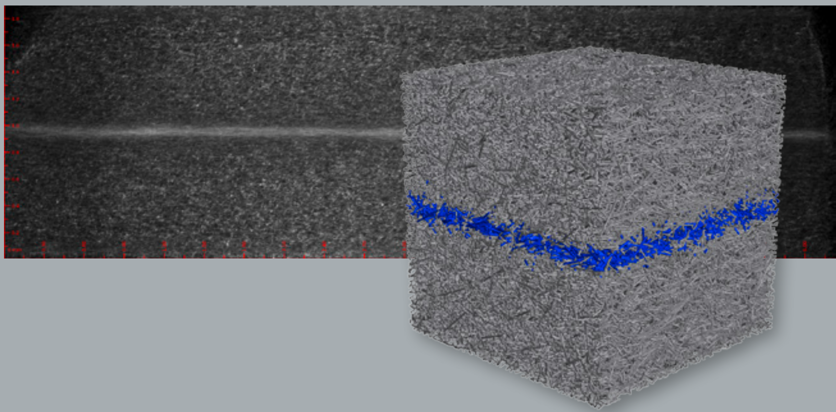
MAIN TOPICS

- Technical Textiles and Nonwovens
- Virtual Material Design and Microstructure Simulation
- Lightweight and Insulation Materials
- Filtration and Separation
- Complex Fluid Dynamics and Multiphase Flows
- Electrochemistry and Batteries



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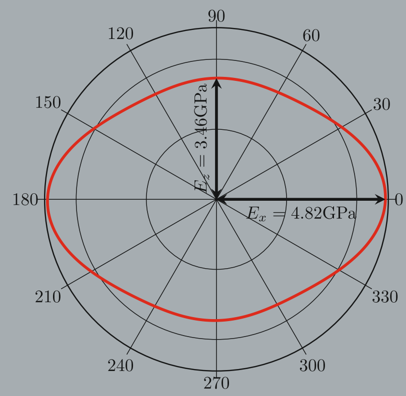

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MULTISCALE SIMULATION OF FIBER REINFORCED COMPONENTS

1 *µCT image of short glass fiber reinforced PBT with characteristic middle layer*

2 *Computer model of a short glass fiber reinforced PBT, generated with the software tool GeoDict*

3 *Computed effective stiffness in thickness and longitudinal direction*

Fiber reinforced plastic components are essential in different applications as e.g. in automotive or medical engineering. In the project MuSiko we develop multiscale simulation techniques for reinforced components.

For microstructured materials, the macroscopic deformation and failure behavior significantly depends on the microstructure, which is influenced by the manufacturing process.

For fiber reinforced polymer matrices as for example polybutylen terephthalat (PBT) matrix failure, fiber breakage or delamination may occur. In order to predict these effects often a pure macroscopic analysis is not sufficient. Thus, very complicated phenomenological models are required, which are only valid for certain failure scenarios.

Joint research project MuSiKo

In the BMBF joint research project MuSiKo we develop efficient multiscale simulation techniques in consultation with scientists from the universities of Kaiserslautern and Saarbrücken as well as the Karlsruhe Institute of Technology. The abbreviation MuSiKo stands for "Adaptive Approximation Techniques for the Multiscale Simulation of Nonlinear Composite Behavior". The industry partners Robert Bosch GmbH and Siemens PLM Software are supporting the research project.

The applied multiscale approach is based on a coupled solution of the macroscopic and the microscopic problem. Only the characteristics of the matrix the fibers as well as the local orientation of the fibers have to be determined as input parameters for the simulation. The mechanical behavior at the level of component results in the averaged microscopic values.

Process chain for glass fiber reinforced plastics

In the project MuSiKo which has successfully been finalized in 2017 we carried out the complete process chain for glass fiber reinforced PBT in cooperation with our partners – from the measurement of the plastic properties and the determination of the fiber orientation by means of µCT up to the multiscale simulations. The simulation results are validated via suitable experiments at the component level.

With assistance of these simulation techniques, it is possible to optimize the injection molding process (e. g. the temperature or injection point) with regard to the functionality of the components.

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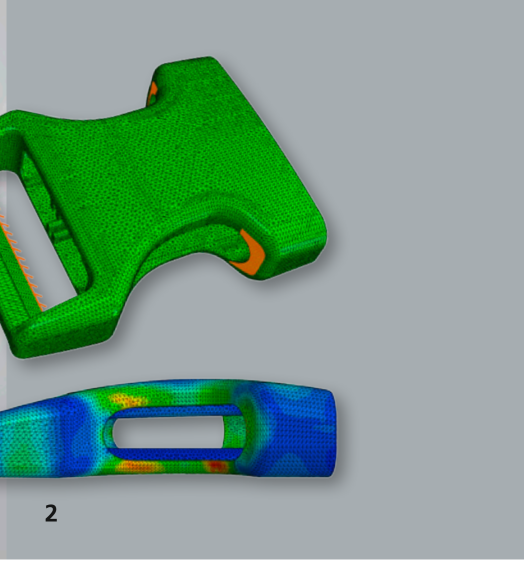

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AUTOMATIC DERIVATION OF MATERIAL LAWS FOR SIMULATING STRUCTURAL COMPONENTS

Fiber reinforced plastics have a high stiffness to weight ratio and can be produced cost efficiently on a mass production scale by injection of compression molding. Therefore, this type of material plays an important role for producing lightweight components. In joint projects with Bosch, we developed an integrative simulation for the dimensioning of short fiber reinforced components, which takes into account the production process as well as the resulting locally varying material properties.

During the production process the plastic is injected or molded at medium to high pressure into the component shape. The resulting flow processes are influencing the fiber orientation and thus the mechanical properties significantly.

Integrative Simulation

At first, a material database for different fiber orientations is filled during the so-called off-line phase. This stage is relying on a combination of microstructure simulations performed with FeelMath and model order reduction methods. FeelMath is a fast and easy analysis tool for elastic micro-structures given by volume images (e. g. CT-Images) or analytical descriptions. Afterwards, the results of the injection simulation with FLUID, Moldflow or Moldex 3D are transferred onto the Finite Element Mesh (FE-Mesh) of the component simulation.

During the component simulation with Abaqus we interpolate the effective material laws obtained during the off-line phase and take account of the local nonuniform mechanical properties. This allows us to take advantage of the lightweight capabilities of fiber reinforced plastics and to avoid overly large safety factors.

1 *Example of a fiber-reinforced plastic part: the buckle of a lanyard*

2 *Above: Boundary condition of Abaqus simulation; below: von Mises equivalent stresses obtained from Abaqus simulation*

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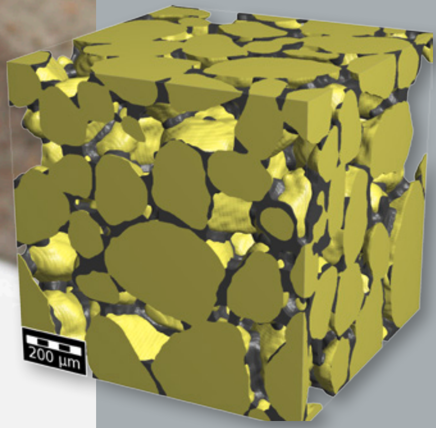

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µ-KERN: MICROSTRUCTURE-BASED CALCULATION METHOD FOR CORE SAND

1 *The sand core was produced by a core shooting process at the UTG. The grains of sand are bound to a mould by a binder.*

2 *Sand grains in beige and binder in grey can be seen in the virtually created microstructure.*

Casting technology uses core sand to map the cooling channels in a cylinder head. Core sand consists of the granular material quartz sand formed to a porous composite by a binder. This is placed in the outer mold before the metal is poured and destroyed after the casting process to produce a sand-free casting. We are developing micromechanical simulation models for core sand in cooperation with the Chair of Metal Forming and Casting (UTG) at Technical University of Munich (TUM).

Calculating the properties of inorganically bound core sands

An innovative, inorganic silicate-based binder complies with strict environmental laws and enables sustainable, low-emission production. However, changing the components used changes the physical behavior of the core sand and the result is only visible after passing through the entire process chain. We are able to accelerate development by modeling and simulating the process.

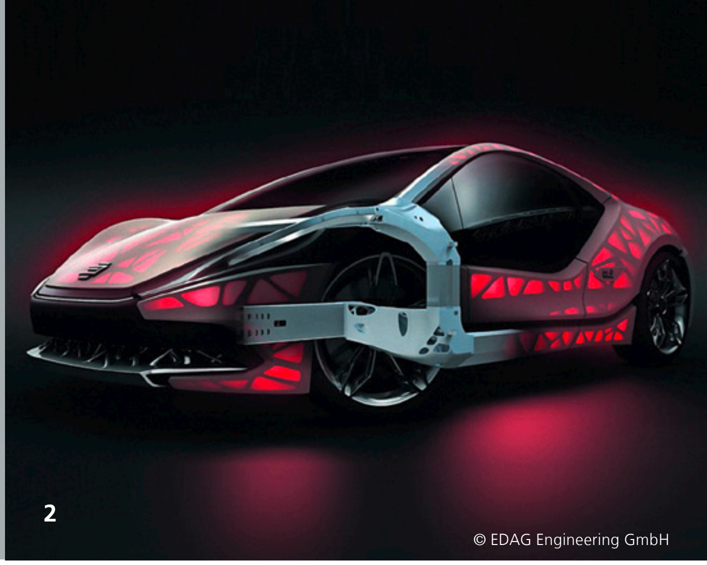
Based on input parameters such as the manufacturing process and the materials used, we effectively calculate physical properties such as strength, gas permeability, and thermal conductivity. In the first phase of the project, we create a representative microstructure for the sand-binder composite and prepare high resolution images of existing composite structures using microcomputer tomography.

Validating the structures produced

The UTG partners measure the elastic properties of the sand and the binder. Then, we create virtual microstructures with stochastic methods and validate them by comparing them with structural images. The properties of the sand (such as grain shape, size, and size distribution) and of the binder (such as volume content and chemical composition) influence the physical properties of the composites. We investigate the dependence of the elastic stresses in the composite on the elastic properties of the materials used i. e., the quartz sand and water glass.

In the second part of the project, we use the Stokes/Navier-Stokes model to calculate the gas permeability and the thermal conductivity. Furthermore, we generalize the elastic model to nonlinear damage effects.

1 © Fraunhofer ILT, Fraunhofer IPT



2 © EDAG Engineering GmbH

MODELING AND SIMULATING ADDITIVE MANUFACTURING BY SELECTIVE LASER FUSION

Additive manufacturing processes have become an integral part of the production of small-batch size, high-stress components such as blades or fuel nozzles for gas turbines. Besides aerospace, automotive manufacturing is predestined for the use of additive manufacturing methods because of the large variety of products. In the BMBF-sponsored project “CustoMat3D”, we develop simulation methods in this area in cooperation with our partners.

New options and degree of freedom in design

The basic principle of additive manufacturing is the layer-by-layer manufacturing process, which eliminates many design limitations due to traditional production methods, like pre-determined tool paths or draft angles. This allows to make full use of the potential of end-use specific lightweight construction as structural components need no longer be of a generic design covering all possible load cases.

Today’s aluminum alloys are generally not customized for a specific application and do not fully exploit cost and weight reduction potentials. Simulations reveal the interplay of material properties, design, and manufacturing processes. However, the optimal simulation approach is still the subject of ongoing research.

Custom aluminum materials for the automotive industry

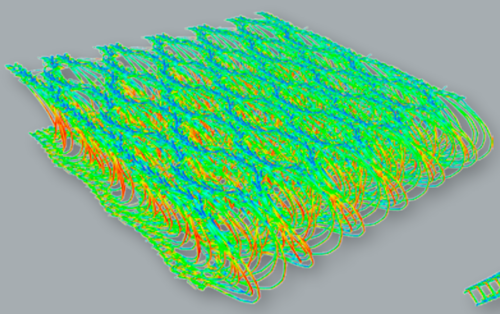
Partners in the CustoMat3D project are: Daimler, Concept Laser, MAGMA, Fraunhofer IAPT, ECKA Granules, FKM Laser Sintering, Institute of Materials Science (IWT), and Altair Engineering. The project is funded within the BMBF project and research scheme “ProMat_3D”. The project´s aim is to use simulation-aided development and qualification to create custom-made aluminum alloy materials for use in laser additive manufacturing for the automobile industry.

In cooperation with MAGMA, we are developing new approaches to simulate the extremely fast phase transitions and solidification process as well as the resulting material structures. To predict deformation, we take into account all relevant length and time scales. Specifically, we include:

- The details of the powder and melt pool in the vicinity of the laser.
- The effects of the punctiform influx of heat due to the laser on the residual stress and temperature distribution throughout the component.

1 *In selective laser melting, the portion of the powder layer belonging to the component is melted first and then the contour is traced for a better surface quality.*

2 *The car bodies of tomorrow are not only lighter, but above all highly flexible in design. The EDAG Light Cocoon concept car demonstrates the new possibilities of structural optimization opened up by additive manufacturing methods.*



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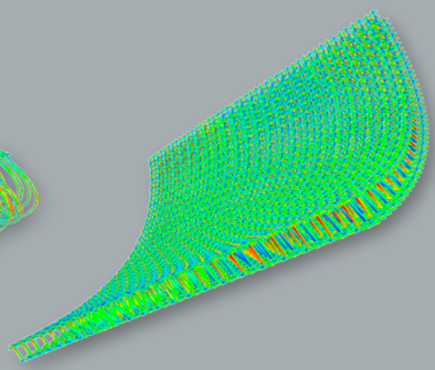

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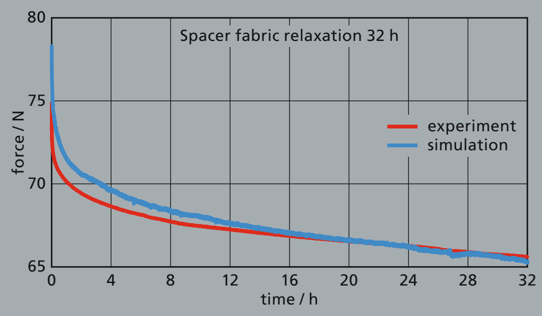

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SIMULATING THE MECHANICAL PROPERTIES OF KNITTED SPACER FABRICS

1 *Compression calculation of a spacer fabric*

2 *Bending calculation of a spacer fabric*

3 *Comparison of simulated and measured relaxation curve of spacer fabrics under compression*

Spacer fabrics are double knit textiles, in the form of plates or shells that consist of two separate layers of knit fabrics joined by vertical monofil yarn. We simulate spacer fabrics in various projects, for example, the areas of application include the materials used in mattresses and seats.

The properties of spacer fabrics are characterized by diverse parameters, such as the in-plane period, the thickness, and the height of the fibers. We can calculate, for example, the effective stiffness and permeability. To reduce the computing effort, we use algorithms for homogenization and dimension reduction. The spacer fabric is represented by an equivalent, elastic, two-dimensional shell.

The resolved microstructure is stored for use in the flow simulation to calculate the effective permeability. The relationship between the geometric parameters and the load determines how much bending or tension is placed on the fiber at the micro level.

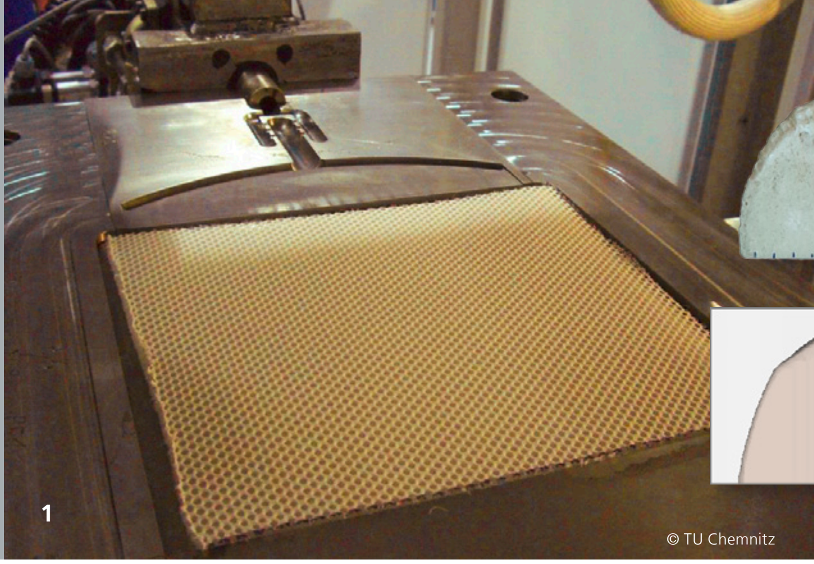
Spacer fabrics are highly resilient, flexible, and strong

One advantage of spacer fabrics is their superior decompression. This means these materials are highly resilient, flexible, and strong when subjected to an external pressure load. In the simulation process, we first build the complex structure of the spacer fabric, resolving all the bonds of the spacer filaments. Subsequently, we simulate the tensile, shear, compression and bending properties using TexMath – software we developed for modeling and analyzing textile fabrics.

DFG Project: Modeling the structural properties of 3D spacer fabrics

The characteristics are generated from the knitting pattern and the yarn's known force elongation curve, cross section, and frictional properties. Using TexMath, we analyze the textile spatial variations of permeability in different directions caused by the outer-plane compression of the structure. This is also a part of a collaborative project with the Technical University of Dresden with the name "Modeling of mechanical and filtration properties of 3D spacer fabrics" and funded by the German Research Foundation (DFG).

Another research question is to what degree the fiber torsion contributes to the overall effective viscoelastic properties. Our investigations show that the relaxation time of the spacer fabrics coincides with the relaxation time of the monofil, as presented in Fig. 3.



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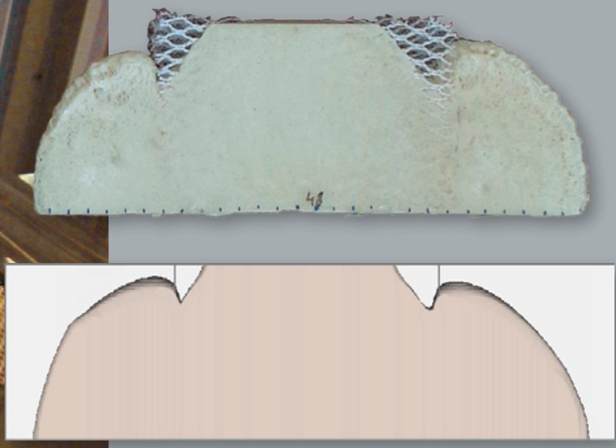

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RIM PROCESS OF POLYURETHANE FOAMS TO DEVELOP COMPOSITE MATERIALS

Composite structures are considered to be lightweight and stable. Textile reinforced composites materials made from polyurethane (PU) foams are perfect candidates due to their enhanced physico-mechanical characteristics. Using FLUID software module of our CoRheoS simulation platform, we can simulate the form filling process.

1 *RIM process of a PU foam with spacer fabric*

2 *Comparison of the filling fronts in an infiltration study*

PU foams are complex and difficult to study

In the RIM process (RIM - Reaction Injection Molding) of PU foams, a polymer mixture is injected into a mold in which the material develops over a period of time from a low molecular weight emulsion to a complex polymer foam matrix via polymerization.

The expanding foam exhibits complex physical behavior during the production phase, which is initiated by premixing adequate reactants followed by gas and heat creation as well as evolution of material properties resulting in PU foam formation. This makes PU foams extremely difficult to study.

Developing optimal simulation tools for industrial applications

We design mathematical models that describe the dynamics of expanding foams and apply them to study the RIM process of PU foams. Using our FLUID software, we carry out relevant numerical studies to understand and evaluate the foam expansion process. In this way, we are able to predict the required amount of material to completely fill the mold as well as optimize the foam process and mold design.

In order to investigate the expansion process in textile structures, especially, knitted spacer fabrics, we use TexMath to determine the relevant permeability tensors. TexMath is an in-house developed software product for the modeling and analysis of textile materials. The spatial variations of the tensors caused by unequal compression of the structure can be analyzed by TexMath (see left page).

We then use this data in FLUID and extend our numerical studies to predict the foam expansion through knitted textiles. Our findings (see figure) are in strong agreement with the experimental data obtained at the Department of Lightweight Structures and Polymer Technology at Chemnitz University of Technology. In summary, we provide simulation tools for efficient industrial application that help in the optimization, manufacturing, and development of composites.

NEWS

BATTERYDICT – BEST MEETS GEODICT

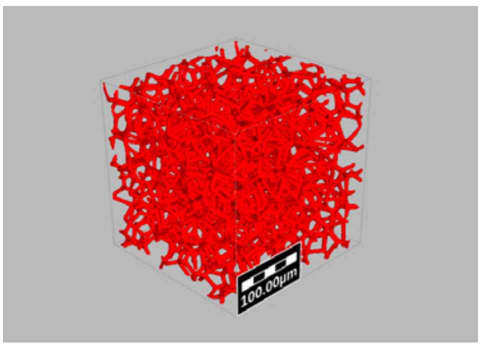
Our cooperation with M2M (Math2Market) was significantly strengthened in 2017 in the area of battery simulations to more closely integrate Fraunhofer ITWM's BEST (Battery and Electrochemistry Simulation Tool) with GeoDict from M2M. This cooperation has produced the new GeoDict module "BatteryDict," which controls the BEST solver algorithms and is completely integrated into GeoDict 2018. Today, in addition to the stand-alone battery simulation software BEST, the software is also completely integrated in GeoDict. We presented BEST and BatteryDict to an interested customer audience and special "short courses" explained the practice in detail at the GeoDict User Meetings in Kaiserslautern, Nagoya, and Tokyo in autumn 2017.

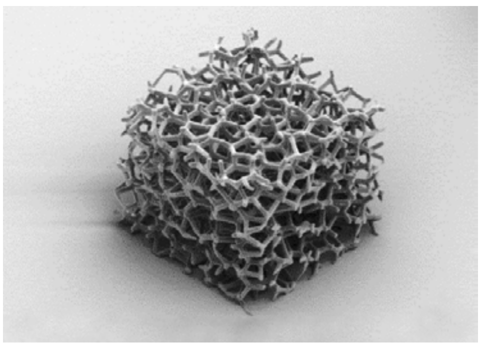
INTEGRATION PROJECT – DIGITALIZATION OF TERAHERTZ TECHNOLOGY

We focus on the experimental qualification of microstructures within the framework of an integration project with the Center for Materials Characterization and Testing. It serves to expand the business areas and promote long term cooperation.

Numerical models and their advanced development are validated on the basis of experimental results to review forecasting reliability. We use the computer to create an optimal microstructure based on the desired material properties, for example, a certain permeability within a specified stiffness.

The 3D printer creates an exact copy of this computer model with (sub-)micrometer resolution, which is then tested for the desired properties. Until now, only indirect verification of microstructure simulations was possible. The success of our explicit validation of additive microstructures creates customer trust and promises new markets.





Front, left to right: Ruturaj Deshpande, Dr. Olena Sivak, Pavel Gavrilenko, Junfan Zhang, Dr. Ehsan Afrasiabian, Dr. Konrad Steiner, Inga Shklyar, Dr.-Ing. Tobias Hofmann, Dr.-Ing. Sarah Staub, Stephan Wackerle, Alexander Leichner, Christine Roth, Dr. Ralf Kirsch, Dr. Julia Orlik, Dr. Ikenna Ebubechukwu Ireka, Dr. Hannes Grimm-Strele, Dominik Gilberg, Dr. Torben Prill, Michael Hauck, Dr. Stefan Rief, Dr. Stephan Kramer, Dr. David Neusius, Dr. Heiko Andrä, Dr. Sebastian Osterroth, Dr. Aivars Zemitis, Jonathan Köbler, Thomas Palmer, Dr. Jochen Zausch, Dr. Dariusz Niedziela