

Table of contents

Nr.	Name	Title	Page
1	Rostislav Daniel	Functional thin films for advanced microelectronics	2
2	Mitterer Christian	Funky surfaces	3
3	Schalk Nina	Advanced surface engineering	4
4	Kostoglou Nikolaos	Advanced characterization of nanoporous materials	5
5	Maier-Kiener Verena	Scale bridging mechanical testing under extreme conditions	6

Functional Thin Films for Advanced Microelectronics

at the Chair for Functional Materials and Material Systems

Our research in thin films for modern microelectronics is dedicated to enhancing the reliability and performance of miniaturized components and devices, focusing on diverse applications including flexible and wearable devices, displays, sensors, and thin film capacitors for energy storage. Besides the development of new functional materials, we prioritize optimizing mechanical stability, thermal management, and stress mitigation within thin film structures through advanced microstructural design and architecture.

We employ innovative techniques in interface engineering to control diffusion processes and enhance adhesion, while exploring opportunities for surface functionalization through the incorporation of nanoparticles and structural features across multiple length scales.

Unique compositions and microstructures by advanced combinatorial approaches

Plasma-assisted deposition and surface modification methods

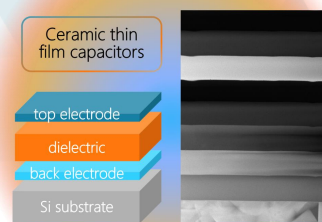
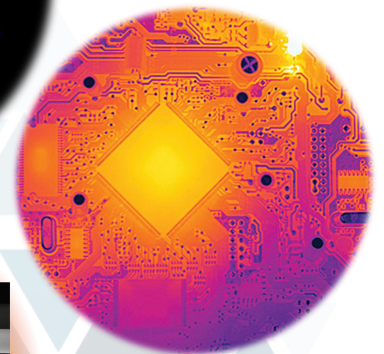
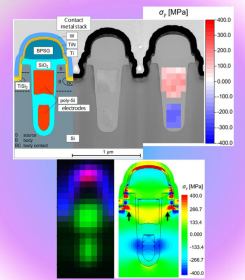
Thermal and stress management by smart architectures and gradient compositions

Functionalization of surfaces

Accelerated process and materials development by high-throughput materials synthesis and characterization

Interface engineering for mechanical reliability and enhanced adhesion

Advanced nanoscale characterization by electron microscopy, Raman spectroscopy, X-ray diffraction and atom probe tomography



Materials Science

By fostering interdisciplinary collaboration, conducting rigorous experimentation, and advancing methodologies, our goal is to actively contribute to transformative advancements in microelectronics.



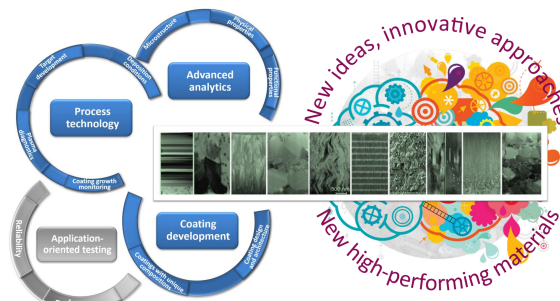
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Advanced Surface Engineering

Scanning Electron Microscopy (Inset: 1 μm)

Electron Back Scatter Diffraction (Inset: 1 μm)

Atom Probe Tomography (Inset: 20 nm)

Workpiece

Cutting Insert

Cutting Tool

Micro-Mechanical Bending Tests (Inset: 2 μm)

Transmission Electron Microscopy (Inset: 100 nm)

Atom Probe Tomography (Inset: 30 nm)

CERATIZIT GROUP

Christian Doppler Forschungsgesellschaft

The focus of the Advanced Surface Engineering group is on the development of processes and materials for multifunctional surfaces and their characterization to establish a fundamental understanding of the synthesis – structure – properties relationships. Thin films with thicknesses of a few micrometers, deposited from the gas phase by vapor deposition methods, for example significantly increase the performance and life-time of tools. Surface engineering is a crucial instrument to help protecting our environment, as it allows to save resources and to reduce the use of harmful coolants and lubricants.

Priv.-Doz. Dr.
Nina Schalk
Head Advanced Surface Engineering

Dr.
Michael Tkadletz
Head Advanced Micro- and Nanostructure Characterization

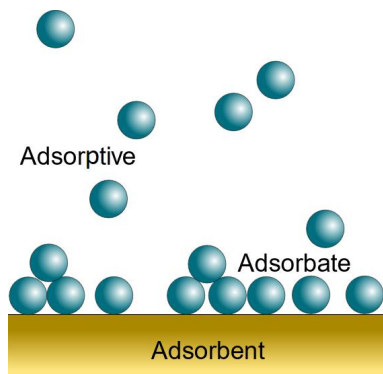
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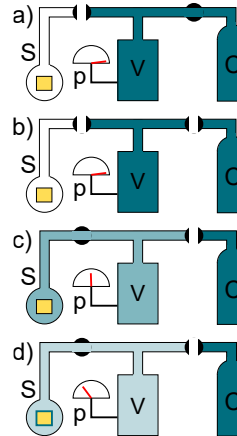
Advanced Characterization of Nanoporous Materials

Physical Adsorption Basics



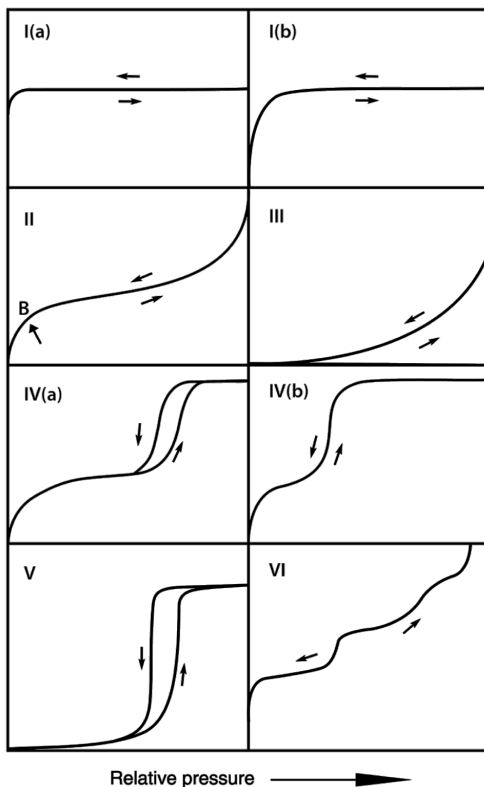
- London dispersion forces lead to an attractive interaction between gas molecules and solid surfaces.
- The resulting change in potential energy of the particles induces a change of the equilibrium phase close to the surface. This causes the formation of an adsorbed layer.
- If the behaviour of the gas is well known, it is possible to get information on the solid surface.

Measurement Principle



- Gas is filled from a storage cylinder (C) into a reference volume (V).
- The valve between C and V is closed, the pressure (p) is recorded.
- The valve to the sample environment (S) opens. The larger volume leads to a p drop.
- The adsorption takes particles from the adsorptive, which leads to an additional p drop. This additional p drop is proportional to the adsorbed mass.

Classification of Isotherms



The shape of the adsorption/desorption isotherm depends on the properties of the gas (**adsorptive**), the solid (**adsorbent**), the adsorbed substance (**adsorbate**) and the amount of adsorbate. It can be used to classify the isotherm and thereby to identify the nanopore (< 100 nm) structure. The isotherm types according to the International Union of Pure and Applied Chemistry (IUPAC) are:

- I(a): Ultra-microporous system with pores smaller than 1 nm. The limit in uptake is controlled by micropore volume.
- I(b): Microporous system (< 2 nm) with few small mesopores (up to 2.5 nm).
- II: Non-porous or macroporous (> 50 nm) surfaces. Point "B" indicates monolayer formation. A more gradual slope is caused by simultaneous onset of multilayer formation. No saturation plateau is reached.
- III: Weak interactions between adsorbent and adsorbate. The molecules form clusters at favourable sites, but no film is formed. No identifiable monolayer formation at low relative pressures (i.e., no point B).
- IV(a): Mesoporous system (2-50 nm). The initial shape is identical to Type II, but at higher pressures pore condensation occurs for larger pores. The final amount of adsorbed material is finite. The width of the hysteresis loop depends on the adsorption system and temperature. It is observed for mesopores exceeding a critical size.
- IV(b): Similar to Type IV(a) but without hysteresis loop, as observed in smaller pores.
- V: Similar to Type III at low pressures but mesoporous behaviour. At higher pressures, the pores are filled.
- VI: Layer-by-layer adsorption on non-porous, highly uniform surface. The height of the steps depends on the capacity of a monolayer.

Thommes et al. (2015), *Pure Appl. Chem.*, **87(9-10)**, 1051-1069



Dr. mont.

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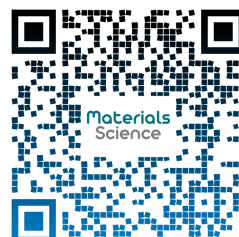
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- ❑ **Research interests:** Nanoporous Materials for Green Energy, Environmental and Biomedical Applications
- ❑ **Partners:** Chair of Physics

Materials Science



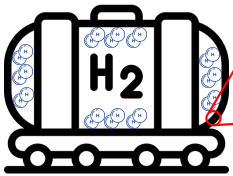
Scale Bridging Mechanical Testing under Extreme Conditions

The development of modern high-performance materials requires a comprehensive analysis on multiple levels. Understanding complex microstructures and their influence on mechanical properties is crucial. For this purpose, we integrate nanoindentation and other micromechanical experiments with macroscopic compression and tension tests to characterize thermally activated deformation processes across various scales. Subsequently, we correlate these data specifically with high-resolution

structural and chemical analysis techniques such as SEM, EDX, EBSD, TEM, and APT.

The results of these investigations enable us to establish reliable mechanistic models that describe the predominant deformation mechanisms of high-performance materials under realistic loading conditions. Our research efforts are conducted in close collaboration with a wide range of international industrial and academic partners to advance the development and application of these materials.

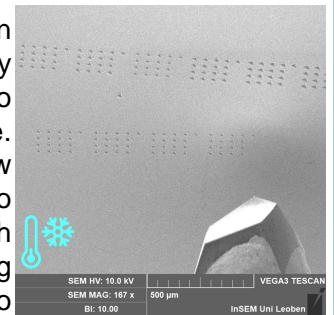
INNOVATIVE



The energy transition is increasing the demand for sustainable energy sources such as hydrogen. However, in contact with certain metals, hydrogen can lead to harmful changes in the mechanical properties, which need to be investigated in more detail. This is partly relevant for applications in the field of hydrogen storage. It is crucial to understand the processes that lead to these property changes in order to be able to design components safely.

COLD

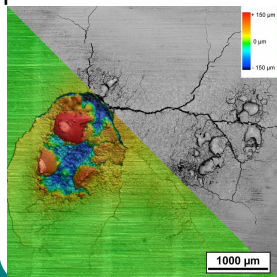
Certain types of hydrogen storage systems require very low operation temperatures to ensure efficient storage. Unfortunately, these low temperatures can lead to embrittlement of materials. With the help of our testing equipment, it is possible to analyze these mechanical properties down to -150°C in order to understand the changes that occur and take them into account accordingly.



HOT

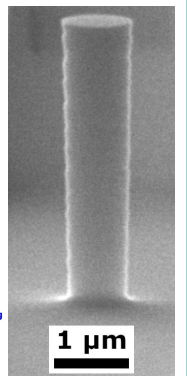
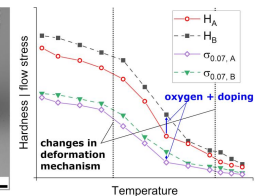
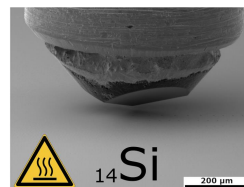
Investigating damage resistance at up to 3000°C :

By exploring novel approaches we aim to push the boundaries of state-of-the-art high-performance materials even further. This is done by controlled electron beam exposure to mimic conditions mimicking or exceeding those in fusion reactors and other cutting-edge applications



SMALL

On the micro- to nanoscale materials react differently to mechanical loading compared to the macroscopic world. Accordingly, mechanical characterization on these length scales is an important field of research and essential to acquiring application-relevant data. Applications that deal with such scale effects are increasingly important, especially in the semiconductor industry.



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