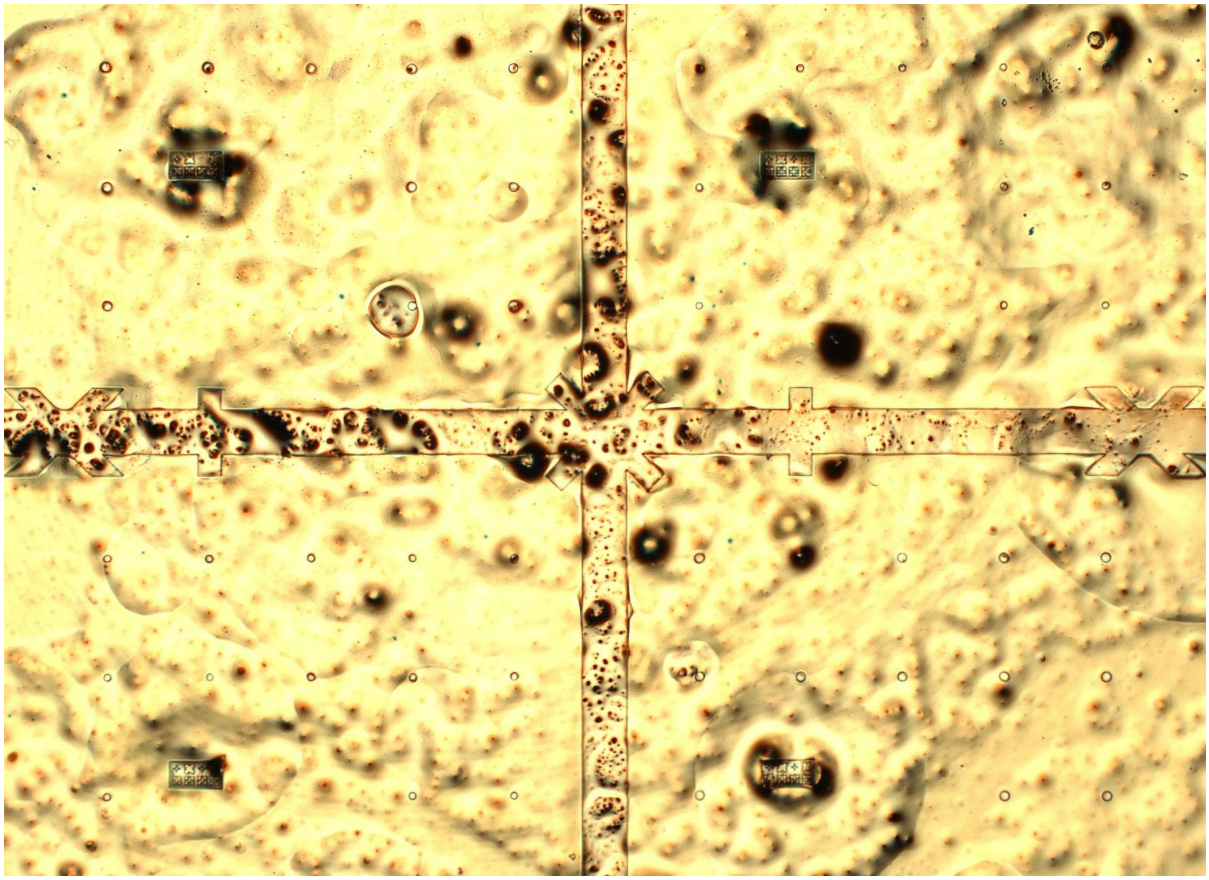
CINSaT

Center for
Interdisciplinary Nanostructure
Science and Technology

Newsletter No. 11 (December 2021)



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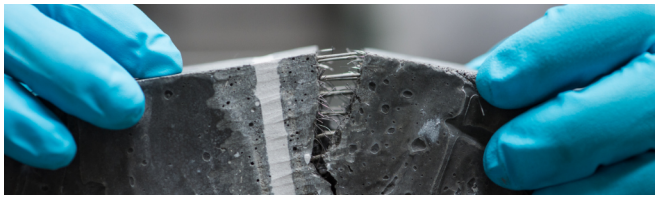

Cover Image

Dr. Daniel Merker, Technical Physics:

Etch tests for microchannels (200 µm diameter) in a quartz glass substrate. The channel structure was defined by optical lithography, deposition of 30 nm chromium, 400 nm gold and subsequent lift-off. Etching was performed with 40% hydrofluoric acid. In spite of the hard mask the covered parts of the glass substrate was also etched by diffused fluor ions.

Preface

Dear reader,

welcome to the second CINSaT newsletter of 2021. Already the fourth newsletter published during the on-going pandemic. However, the increasing number of vaccinated people made it possible to relax the hygiene rules of the University of Kassel to some extent, which enabled the CINSaT to organize the annual autumn colloquium in the form of presence again. The autumn colloquium was held on 3rd of November 2021 in lecture hall 0282 of the AVZ with special admission rules in effect, only allowing vaccinated, recovered or people with a current test to participate and mandatory face masks. Despite these restrictions the autumn colloquium was well received with over 100 participants who listened to four interesting scientific talks. Afterwards the poster session was held with over 50 poster contributions shared while enjoying the buffet. You can read more about the autumn colloquium in the Latest Report section.

It is very pleasant that I can inform about very recent decision of DFG. The DFG cooperative research project ELCH was approved for further 4 years. Also recently the DFG decided that the student training school on “Biological Clocks on Multiple Time Scales” will be funded and will start in January 2022. Congratulations to the responsible speakers “Thomas Baumert” and “Monika Stengl” and their teams for this great success. Several contributions to these topics will be reported also in this issue.

From 26th of October to 1st of November 2021 the majority of the CINSaT members participated in the shooting of the CINSaT films. On five days a photographer, a cinematographer and a sound engineer visited the participating members in their bureaus and laboratories recording raw material for the creation of the CINSaT films and image photographs that will shape the public presentation of the CINSaT in the following years to come. A small impression of the shooting will be given in the Last Reports section as well. This should also remind you that we are facing next year the 20th annivisary of CINSaT, which we want to celebrate hopefully with no or reduced impact by the Pandemy. The planning has already started. Contributions by all members are very welcomed.

Thanks to the numerous contributions of our members, we were able to create an interesting newsletter once again. In total five scientific publications of our members will be presented in this issue. Prof. Dr. Demekhin in collaboration with Prof. Dr. Ehresmann presents a work on fourfold differential photoelectron circular dichroism. A comprehensive review article on nanophotonic sensors is presented by Prof. Dr. Hillmer. Prof. Dr. Popov reports on proteome studies on cells grown on thin diamond films and Prof. Dr. Fuhrmann-Lieker is presenting two publications about chiral nanostructures in azo polymers and the multigeneration clock in diatoms.

Additionally, three new projects are introduced. Prof. Dr. Heim presents a DFG project to develop a model for the electrical contact resistance at metal-plastic interfaces. Prof. Dr. Middendorf’s new DFG project aims for an elementary physical and chemical bridging model for the initial dissolution mechanism of cement clinker hydration connecting the nanoscale to the microscale level. Priv. Doz. Dr. Benyoucef reports in collaboration with Prof. Dr. Popov about a new BMBF project involving over 25 universities, research facilities and companies with the goal to implement novel quantum repeaters and test their operations in real conditions.

Like always, I hope you enjoy the reading of this issue and stay healthy!

General

Latest information from the CINSaT management

Here we report briefly about key issues from the CINSaT committees, important discussions, and decisions from their meetings.

New Focal Point – Nanomaterials created

Although no meeting was held in either of the committees of the CINSaT, the first vote-by-mail was conducted in October, which was enabled by a corresponding paragraph added to the CINSaT regulation in June this year. The voting was initiated by our members Prof. Dr. Middendorf and Prof. Dr. Niendorf who proposed the renaming of the CINSaT focal point 6 „Nanostructures in natural sciences, engineering sciences and the arts". The initiators argue that material sciences have developed into a major focus for the University of Kassel and the CINSaT, which should be addressed by the creation of a dedicated focal point. In an informal meeting of the Scientific Coordination Committee the issue and possible new names were discussed. The name „Nanomaterials" was chosen and submitted to the members for voting. The new Focal Point Name was approved by 22 out of 25 valid votes (2 nos and 1 abstention).

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Research Highlights

Nanophotonic sensorics: methodologies, resolution and miniaturization limits

Recently, we published an invited review article in PHOTONICS [1], comparing different sensor principles regarding minimum potential size limits, selectivity, sensitivity, resolution, spectral tuning ranges, and efficiency. We discussed that these demands are often difficult to optimize simultaneously since they are oftentimes counteracting each other.

Miniaturizing classical grating spectrometers would mean reducing optical path lengths and the number of illuminated grating lines, yet both will result in decreased spectral resolution. Although there are alternatives to maintain resolution despite miniaturization, they are only possible on the expense of reduced intensity per wavelength interval, which is related to efficiency i.e. signal-to-noise ratio. These alternatives reveal fantastic small spectral linewidths, such as interferometric methods like arrayed waveguide gratings (AWG) and Fabry–Pérot (FP) filters, or photonic crystal (PC) sensors and plasmonic sensors. Chirped fiber Bragg gratings (FBG) offer smallest linewidths (FWHM = full widths of half maximum). Using micro-electro-mechanical systems (MEMS), wavelength tunable sensors can be implemented, which offers potential for further miniaturization. Tunable MEMS have been demonstrated for FP and PC sensors. Figure 2 is taken from our review [1] which compares several sensing methodologies and includes many references.

Using MEMS electrostatic actuation the air-gaps can be manipulated, thus allowing the filter wavelengths to be spectrally tuned. The wavelength tuning efficiency $\Delta\lambda/\Delta L$ for InP multiple air-gap MEMS tunable filters (Fig. 1) is found to be the closest to 1 and the tuning span is 221 nm. These filters reveal much smaller size compared to other systems. In our comparison, the tunable chirped fiber Bragg grating reveals by far the largest space requirement but also the smallest linewidth of 0.007 nm at 1.5 µm. The next lowest linewidths (0.1 nm at λ = 1.3 µm) were measured in MEMS tunable PC filters. Potentially, the space requirement is also very small. However, in order to obtain larger spectral spans of e.g., 400 nm, the combination of several neighboring spectral tuning ranges is required. On the other hand, AWGs also provide small linewidths, and the arrangement of several arrays next to each other is easily attainable. The typical linewidths measured for FP filter arrays are higher than the typical values of PC or AWG sensors. A linewidth of 0.1 nm could be achieved at λ = 1.5 µm in an InP/multiple air-gap FP filter (Fig. 1). However, maintaining very small linewidths during tuning are challenging in the InP multiple airgap MEMS technology.

Various static FP filter arrays can be manufactured next to each other within a single 3D nanoimprint step. This technology enables lowest tentative price per spectral range for visible spectral ranges. Plasmonic MEMS sensors evaluate charge carriers induced by the surface plasmon polariton resonance into a diode structure and transform this angle dependent current into the spectral information. Although they reveal rather high linewidths of >10 nm, the assured wide tuning ranges is highly favorable. Thermally tuned chirped FBG shows narrow band filter lines with FWHM of 0.007 nm and can potentially be implemented in any working spectral range of an optical fiber. The small tuning range of only 16.5 nm requires, however, an array of many individual chirped FBG to cover broader spectral spans. The classical grating spectrometer is definitively the best in our comparison in term of the efficiency in making most out of available light. However, the grating spectrometer suffers considerably from strongly reduced spectral resolution in downsizing of the devices, whereas such limitations are not relevant for all the other sensor types compared in our review. In all these cases, the resolution is very high and independent from miniaturization. The AWG uses available light much more efficiently than the static and tunable FP filter arrays and the tunable PC filter array. The latter three own rather low efficiencies, but the efficiencies can be boosted by spectral preselection as shown in this review.

Nanoimprint can be applied to all the compared sensors, except the chirped fiber Bragg grating and the classical grating spectrometer. Transmission gratings could be fabricated by nanoimprint lithography. Nanoimprint technology reveals its full potential in manufacturing static FP filter arrays, in which 192 different filter lines have been demonstrated using a single 3D nanoimprint step to define accurate and diverse 3D cavity layers. There are no limits to considerably increase these values in static FP filter arrays. At the same time, nanoimprint substantially reduces fabrication time, cost and effort.

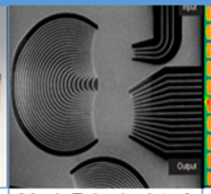
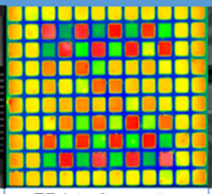
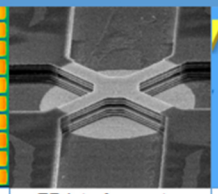
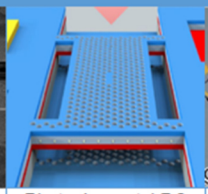
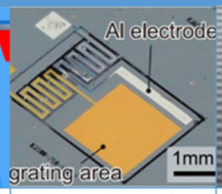
		Mini Spectrometer	Mini Spectrometer	AWG	Static FP filter array	Tunable MEMS FP filter	MEMS tunable PC filter	Plasmonic MEMS Sensor	Tunable Chirped FBG
Miniaturized spectrometers for larger spectral ranges									
Operation principles		Transmission Grating	Reflection Grating	Mach Zehnder interf.	FP interferometer	FP interferometer	Photonic crystal PC	Plasmonic coupling	Grating phase shift
Spectral range		340–830 nm 950–1700 nm	340–850 nm 640–1050 nm	643–863 nm 1530–1565 nm	400–1700 nm	200–2000 nm	1290–1340 nm	550–1700 nm	200–2000 nm
Active tuning range		-	-	-	-	221 nm @ 1.5 µm	30 nm	300 nm @ 1.4 µm	16.5 nm @ 1.5 µm
FWHM Δλ typical values	**VIS**	6 nm	13 nm	0.1 nm	2.5 nm @ 500 nm	2 nm @ 600 nm	-	-	-
	NIR	12 nm	20 nm	0.4–0.8 nm	5–6 nm @ 1.5 µm	3 nm @ 1.5 µm	-	-	-
FWHM Δλ record values	**VIS**	4.3 nm @ 480 nm 4.2 nm @ 725 nm	12 nm @ 420 nm	0.05 nm	1 nm @ 500 nm	1 nm single air-gap	-	-	-
	NIR	-	17 nm @ 950 nm	0.22 nm @ 1.5 µm	5 nm @ 1.5 µm	0.1 nm InP/multi air-gaps @ 1.5 µm	0.08 nm @ 1.3 µm	10 nm @ 1.3µm	0.007 nm @ 1.5 µm
Resolution VIS	**λ/Δλ**	100–170	35–50	-	500	-	-	-	-
Resolution NIR	**λ/Δλ**	~100	42–56	7000 @ 1.5 µm	300	300–15000	3000–10000	100–150	220000
Recording speed		very fast	very fast	very fast	very fast	medium	fast	medium	slow
Production challenge		Automation. The rest are proprietary information	proprietary information; most probably alignment of PD array and blazed grating	to achieve effective refractive index homogeneities in the individual ridge waveguides	perfect resist filling of templates, residual layer homogeneity or effort in individual etching and deposition	flat membranes, vertical stress gradient compensation	QD spatial positioning and adjusting its spectral line, e-beam lithography serial writing	flat cantilever, stress in metal layer, large angle stroke	fabrication of precise chirp in fiber, positioning and actuation of heater element
Nanoimprint applicable		probably	no	yes	yes	yes	yes	yes	no
Potential space requirements to cover	**400nm in vis**	43 mm^2	200 mm^2	90 mm^2	small 0.07 mm^2	small 0.06 mm^2	-	-	-
	500nm in NIR	43 mm^2	46 mm^2	50 mm^2	small 0.09–1 mm^2	small 0.05 mm^2	small 0.33 mm^2	medium 9.5 mm^2	large 300 mm^2
package size	**in vis range**	medium	large	large	small	small	-	-	-
	in NIR range	medium	medium	large	small	small	small	medium	very large
Current and tendative price		600€ PEBBLE vis	500€ C12880MA	high	low	high	high	medium	medium
Yield		100%	high	medium	high	medium	medium	medium	high
Efficiency in available light		very high 70–80%	very high	medium	weak, can be boosted	weak, can be boosted	weak, can be boosted	weak, can be boosted	medium

Fig. 2: The review benchmarks and compares various optical properties, raises the question of benefit in using nanoimprint lithography for the sensor fabrication and estimates the lowest potential required space for a spectral span of 400nm in the visible and of 500nm in the infrared spectral range. λ denotes the vacuum wavelength.

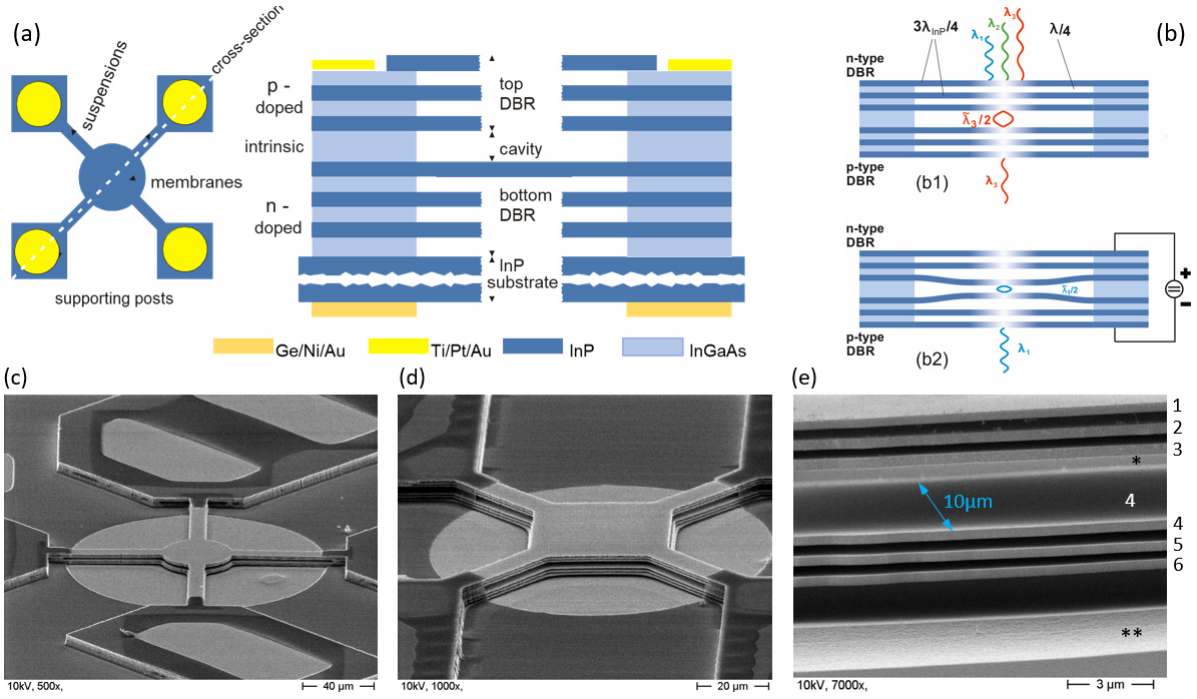


Fig. 1: Schematics and SEM micrographs of InP/InGaAs multiple air-gap MEMS tunable FP filters. Each DBR consists of 3 InP layers and 2 air-gaps. The vertical thickness of the 3λ/4 InP is 357nm and of the λ/4 air-gap is 375nm. The central air-gap is λ/2. (a) (Left) top view on an InP filter element showing four supporting posts with four contact pads (yellow), four suspensions and the top membrane (the top one out of 6 membranes lying below). The orientation of a subsequent cross section is shown by the white broken line. (Right) cross section of the MEMS multilayer structure. InGaAs exists only inside the supporting posts. Between the suspensions/central membrane InP layers, InGaAs was serving as a sacrificial layer and had been selectively removed and replaced by air. The bottom contacts are shown in orange. (b) Schematic of MEMS tunable FP filters including multiple air-gaps and membranes and suspensions made of InP. The supporting posts are built of the complete InP/InGaAs multilayer stack, (b1) unactuated state, (b2) actuated. λ̃ is an effective wavelength, explained in [1]. (c) 60 µm long suspensions and a circular membrane with 40 µm diameter. (d) Square membranes. (e) Details of the suspension region: allowing a view through the structure to the ground behind marked with "". The ground level in front is marked with "**". The three InP layers from top DBR are indicated by 1, 2 and 3. The three InP layers from bottom DBR are indicated by 4, 5 and 6.*

Further information

[1] H. Hillmer, C. Woidt, A. Kobylinskiy, M. Kraus, A. Istock, M.S. Q. Iskhandar, R. Brunner and T. Kusserow: Miniaturized Interferometric Sensors with Spectral Tunability for Optical Fiber Technology - A Comparison of Size Requirements, Performance, and new Concepts. PHOTONICS 8, 332 (2021).DOI:10.3390/photonics8080332

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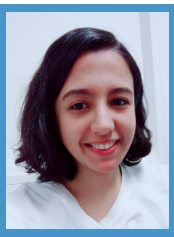

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Implant coating with ultrananocrystalline diamond film could lead to enhanced integration and bone formation

A collaboration between the University of Kassel and the Institute of Molecular Biology, Bulgarian Academy of Sciences demonstrated the advantages of ultrananocrystalline diamond coating on bone implants for better osseointegration

The successful osseointegration, i.e. the fully functional connection of the patient's bone and artificial implant, depends on the response of the cells to the direct contact with the surface of the implant. The surface properties of the implant which trigger cell responses leading to its integration into the surrounding bone can be tailored by surface modifications or coating with thin layers. One potential material for such applications is ultrananocrystalline diamond (UNCD). It combines the exceptional mechanical properties of diamond with good biocompatibility and the possibility of coating as thin uniform films on different substrates of biological interest. The main objective of our study was to determine the relationship between the extracellular matrix (ECM) adhesion of human osteoblast MG63 cells and the substrate surface properties (chemistry, wettability, topography), and to relate their effect on the cellular response and possibility to enhance bone regeneration via UNCD modified titanium implants.

In our work recently published in Materials Science and Engineering C we firstly deposited UNCD films on titanium-coated substrates and applied oxygen or ammonia plasma to modify their surface properties. The as-grown and modified UNCD exhibited relatively smooth surfaces with topography dominated by rounded features. The modifications induced oxygen- or amino-terminated surfaces with increased hydrophilicity. In addition, the UNCD coatings exhibited a very low coefficient of friction when diamond was used as a counterpart. As-grown and modified UNCD samples were applied to study the responses of human osteoblast MG63 cells triggered by surfaces

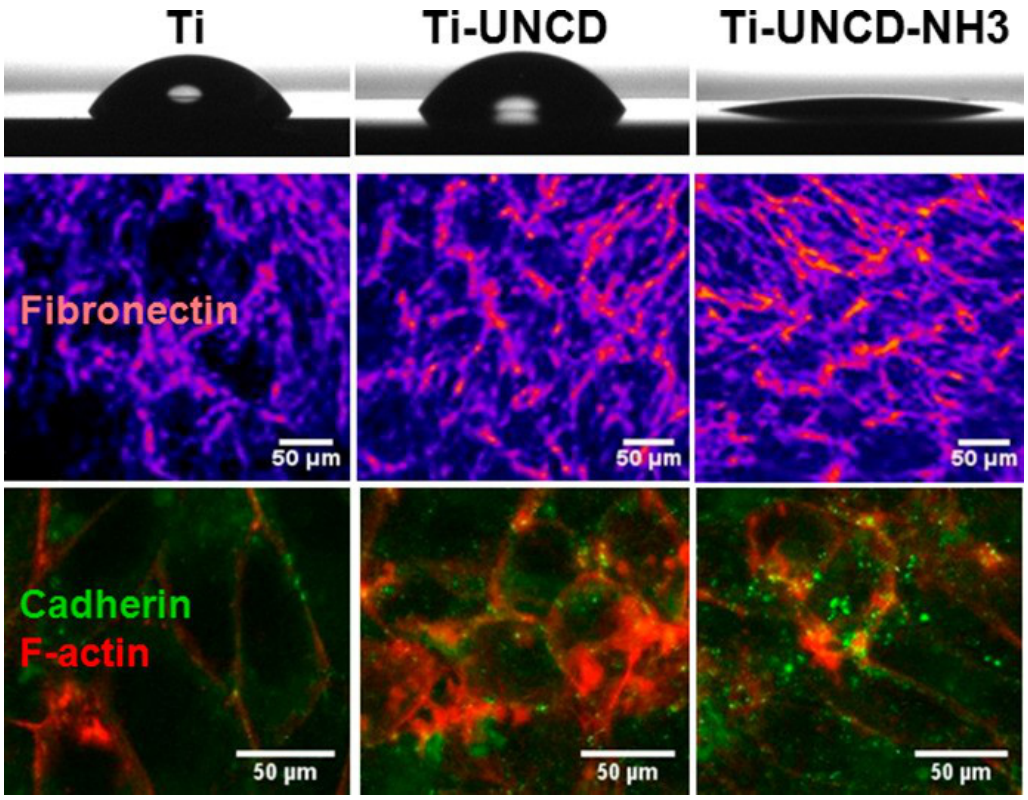

Fig. 1: Immunofluorescence staining for fibronectin, cadherin, and F-actin formation during MG63 growth on Ti, Ti-UNCD, and Ti-UNCD-NH3 surfaces.

with various terminations assessed by proteomic analysis. The results revealed that the coating of Ti with UNCD as well as the plasma modifications resulting in O-or NH_2-terminated UNCD induced upregulation of proteins specific for cyto-skeleton, cell membrane, and ECM involved in the cell-ECM-surface interactions. Proteins from each of these groups, namely, vimentin, cadherin, and fibronectin were further studied immunocytochemically and the results confirmed their increased abundance leading to improved cell-to-surface adhesion and cell-to-cell interactions. These findings demonstrate the potential of implant coating with UNCD and its surface modifications for better osseointegration and bone formation.

Further information

Daniel Merker, Yordan Handzhiyski, Rolf Merz, Michael Kopnarski, Johann Peter Reithmaier, Cyril Popov, Margarita D. Apostolova, Influence of surface termination of ultrananocrystalline diamond films coated on titanium on response of human osteoblast cells: A proteome study, Mater. Sci. Eng. C 128 (2021) 112289, https://doi.org/10.1016/j.msec.2021.112289

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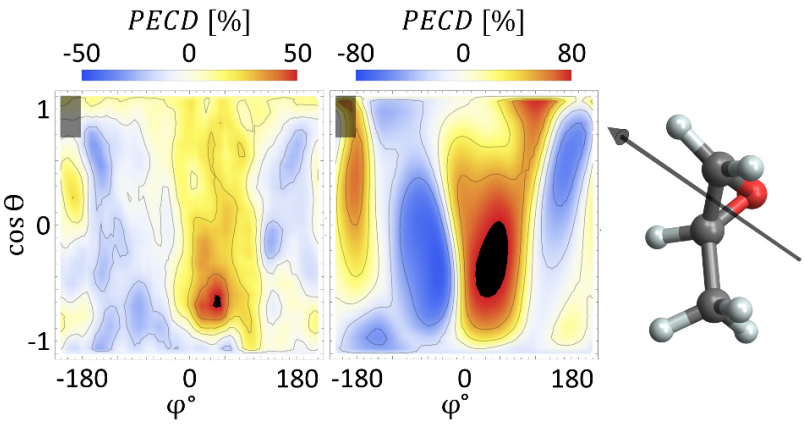
Fourfold Differential Photoelectron Circular Dichroism

Oxygen 1s-photoionization of fixed-in-space methyloxirane molecules with circular polarized light has been studied experimentally and theoretically, and an enhancement of a chiral asymmetry in the angle resolved photoelectron emission spectra clearly beyond 50% is demonstrated.

Photoelectron circular dichroism (PECD) is a fascinating chiroptical phenomenon of the forward–backward asymmetry in the emission of photoelectrons from randomly-oriented chiral molecules irradiated by circularly polarized light. Because PECD is a pure electric dipole effect, it is much stronger than the conventional circular dichroism (CD) in photoabsorption spectra of chiral molecules. For randomly oriented molecules, this chiroptical effect emerges on the level of a few percent, which makes it a well-established tool for chiral recognition in the gas phase. Within the LOEWE focus project ELCH (2013–2016), in a close cooperation with the scientific research groups of Reinhard Dörner and Markus Schöffler (Goethe-Universität Frankfurt) and Robert Berger (Philipps-Universität Marburg), we found that PECD can be enhanced up to about 10-20% by fixing already one molecular orientation axis in space. In the currently running DFG collaborative research center SFB-1319 ELCH, together with the same cooperation partners, we show now experimentally and theoretically that PECD of a fully fixed-in-space chiral molecule can reach a much higher contrast of more than 50%. As is illustrated in the figure below, the differential PECD for S-methyloxirane as a function of the two photoelectron emission angles, measured (left panels) and computed (right panels) for a given molecular orientation (see inset at the right-hand side), exceeds the presently chosen upper/lower limits of the respective asymmetry scales (highlighted by black spots). Our findings pave the way for promoting PECD to an unprecedently-sensitive tool for chiral recognition in the gas phase.



Further information

Fehre et al., Phys. Rev. Lett. 127, 103201 (2021); doi:10.1103/PhysRevLett.127.103201

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The Photonic Drill: Chiral Nanostructures in the Solid State

Birefringent materials have a distinct advantage in comparison to other optical materials: they provide several refractive indices that can be used for the construction of optical nanostructures relying on refractive index contrast. A paramount example is chitin which occurs in the elytra of beetles. In addition to being a firm protection for the wings, it gives rise to a brilliantly coloured appearance due to its layered depositon in different directions. In certain beetles of the scarabaeid family, these layers exhibit a helical twist, resulting in the unique property of selective reflection of circularly polarized light. If you look at such a beetle through typical 3D cinema glasses, you will see a colored beetle through one eyeglass, and a black one through the other. Cholesteric phases of liquid crystals used in thermometer strips are based on the same principle. Here, the colour that is reflected changes with temperature, indicating changes in the pitch of a birefringent helix in the liquid crystal.

In chitin and cholesteric liquid crystals the handedness of the helix is predetermined by the chirality of the underlying molecular components. It would be of interest, however, to design technical photonic components using only achiral molecular components. With such materials it could be easier to control pitch, direction and especially handedness of birefringent helices in three-dimensional nanostructures. Materials that are suitable for this purpose may be azo polymers. In azo polymers, birefringent structures can be induced by molecular reorientation. For this process, the azo polymer is irradiated with polarized light in the overlapping absorption bands of the cis and trans isomers. Being excited and isomerizing from trans to cis again and again, the molecules diffuse out of the orientation of the polarization

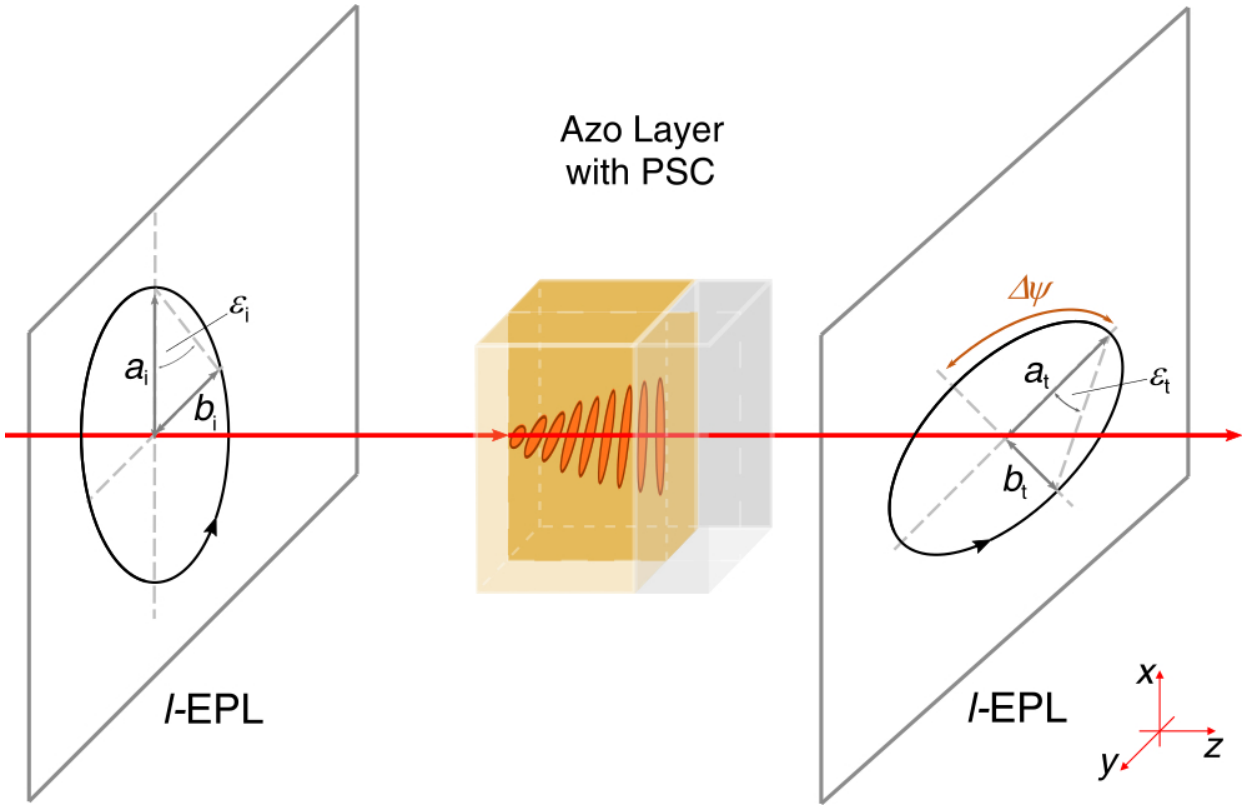

Fig. 1:. Photoinduced Supramolecular Chirality (PSC) in bulk azo materials under irradiance with elliptically polarized light (EPL).

direction and reorient in a plane perpendicular to the incident polarization. This reorientation process results in negative birefringence. But how do the molecules react on circularly or elliptically polarized light? In 2002, the group of D.Y. Kim at Kwang-Ju in Korea reported the induction of supramolecular chirality in amorphous films of azo polymers by irradiation with elliptically polarized light of a certain handedness. The achieved rotation of the optical axis of light following the twist of the helical structure while passing the film was reported to be 4.5°, too low for being of technical interest at that time.

In our recent work [1,2], we employed high-performance azo polymers that are characterized by a high optical anisotropy and achieved record values for optical rotation of 112°/µm. Under the assumption of a wave propagation similar to cholesteric liquid crystals this means that the orientation of the azo groups at the back side of a 800 nm thin film is almost perpendicular to the orientation at the front side. The writing process is dynamic in a timescale of a few minutes, in which the irradiating light wave – after encountering a small symmetry break at the surface – drills itself into the depth of the film. Thus it leaves a rotating trace of birefringent layers and self-induced transparency due to the induced dichroism. With these findings, three-dimensional optical nanostructures come into reach. At the surface of a bulk material, a quarter rotation of a birefringent helix could be used for defining optical waveguides without the necessity of depositing multilayer structures. The additional benefit inherent in the photoreorientation mechanism is that waveguides obtained by this process would be reprogrammable – a unique feature for optical integrated circuits.

Further information

[1] S. Bagatur, T. Fuhrmann-Lieker, "Photoinduced supramolecular chirality and spontaneous surface patterning in high-performance azo materials", J. Europ. Opt. Soc. Rap. Public. 15, 12 (2019), doi: 10.1186/s41476-019-0104-5

[2] S. Bagatur, M. Schlesag, T. Fuhrmann-Lieker, “Polarization Dependent Photoinduced Supramolecular Chirality in High-Performance Azo Materials”, Molecules 26, 2842 (2021), doi: 10.3390/molecules26102842

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A multigeneration clock

The lifespan of organisms is controlled by biological timers that govern the transition of one generation to the next. However, the concept of birth and death is not so clear for unicellular organisms that simply proliferate by cell division. Some organisms though have invented timing systems that allow them to monitor generations in a population beyond the lifespan of individual cells. Thus they control the timescale for cycles in their population that last over many years. We refer to diatoms, a group of unicellular algae, and their multigeneration clock as an intrinsic mechanism caused by the elaborated nanostructured silica cell walls that enclose each cell.

The cell wall of diatoms consists of two halves that fit together like the two halves of a Petri dish. When the cells divide, a new silica shell is constructed within each if the two halves, respectively. Thus, the cell size has to shrink from generation to generation until the cells become so small that they cannot divide further and switch to sexual reproduction. Then the whole vegetative process starts again by providing initial cells of a large size. Field measurements of diatom size distributions in lakes support the idea that this cyclic decreasing-restoration process lasts over hundreds of generations.

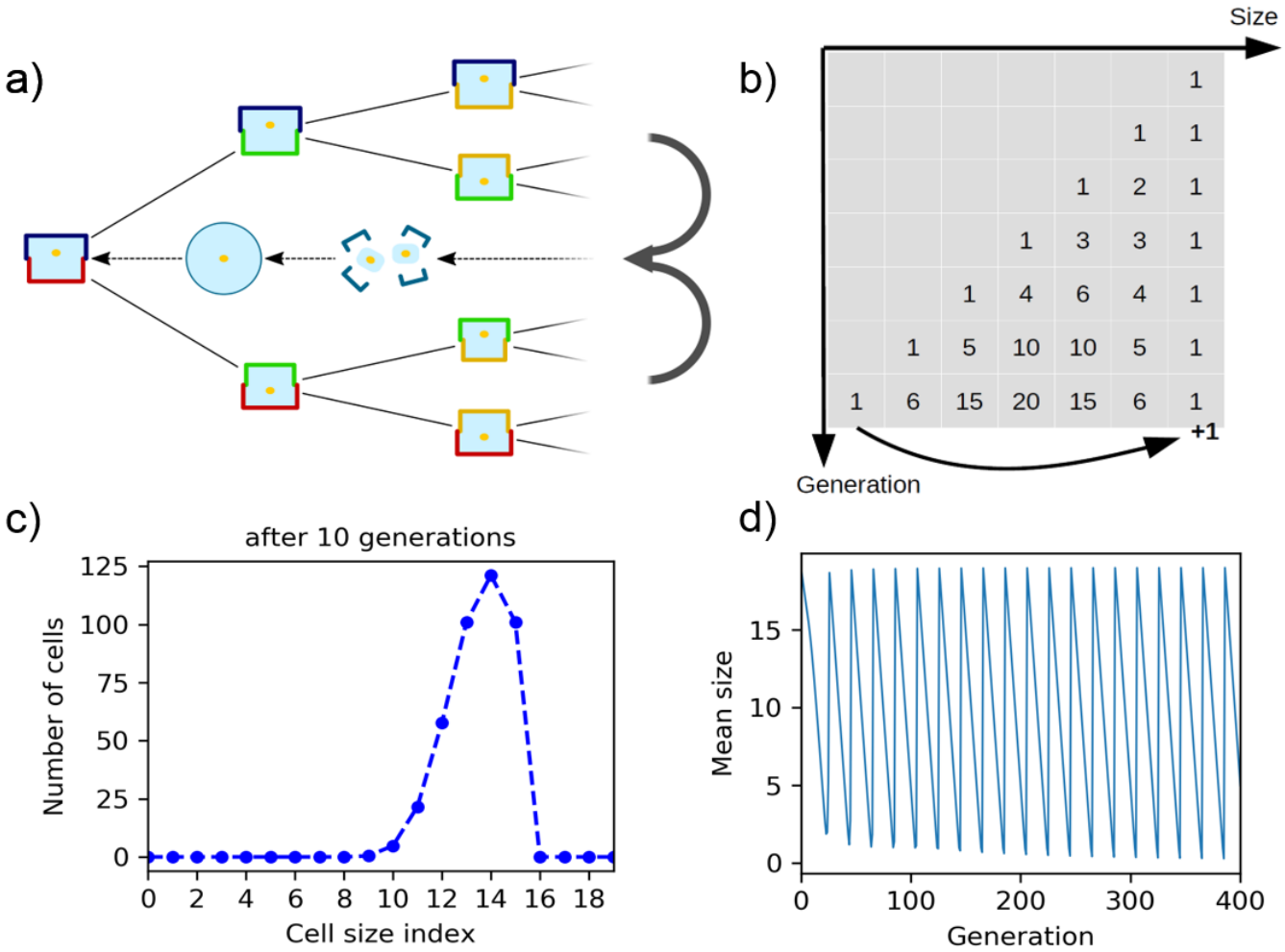

Fig. 1: a) Life cycles of diatoms consisting of a size-decreasing vegetative phase and a size-restoring sexual phase. b) Expected cell size distribution according to Pascal's triangle c) Cell size distribution under ageing d) Long term oscillations in cell size distributions

But wait – there is a caveat: In each division one half retains the parental size. If these halves are accumulated, the cell size decreases on average but on the other hand the cell size distribution widens. By algebraic methods (the Perron-Frobenius theorem, to be more specific) it can be shown that the simple mechanism would never lead to a true cyclic behavior in which the same state of size distribution is regained after a certain period of time. In our recent paper [1], emerged from a collaboration of nanoscientists and mathematicians, we addressed this issue further and asked under which circumstances true limit cycles or at least sustained oscillations can be formed. Nonlinear processes come into mind, but we found an answer in a different direction: Ageing could be the clue, with limited lifespans of individual cells and a potential timing or ageing bias between the two daugther cells in asymmetric cell division. Thus, the fate of the long-cycle clock depends on the timers of a shorter timescale in individual cells. This may not be enough, however, since still there should be a relaxation to equilibrium distributions, albeit in almost geological timespans of millions of generations. But in real ecosystems seasonal changes and environmental fluctuations stochastically influence the reproduction rates and thus continously deflect the clock from a steady path towards stagnancy.

The models and investigations – even if they seemingly address a special feature of special organisms – are important for understanding oscillating behaviour in our complex global ecosystem. Diatoms are not rare – they are responsible for 20-25% of the total carbon fixation on earth. Understanding the population dynamic of diatoms and their blooms therefore is a crucial part for understanding the total carbon dioxide turnover in our world – and this all depends on processes in the nanoscale during each cell reproduction.

Further information

[1] T. Fuhrmann-Lieker, N. Kubetschek, J. Ziebarth, R. Klassen, W. Seiler, “Is the diatom sex clock a clock?”, J. Roy. Soc. Interface 18, 20210146 (2021), doi: 10.1098/rsif.2021.0146

This work is to be continued experimentally in the interdisciplinary DFG-funded Research Training Group "Biological Clocks on Multiple Time Scales", starting in 2022.

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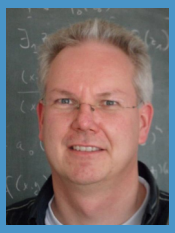

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New Projects

BMBF Research Project: Quantum Repeater Link

The current quantum communication links reach their technological limits when transmitting over long-distances (from about 100 km). To overcome this limit, so-called quantum repeaters are necessary which will connect nodes along a transmission link using quantum memories and simple quantum information processing. They present special quantum physics processing units that receive incoming quantum states and use them for secure communication. Several quantum repeater links can be connected in series which will make it possible to extend the transmission distances to far more than 100 km.

The goal of the joint project "Quantum Repeater.Link (QR.X)", involving 43 partners from 25 German universities, research institutes and companies is the first implementation of novel quantum repeaters and their operation under real conditions. New and innovative approaches will be investigated in three material systems based on trapped atoms and ions, quantum systems in diamonds as well as in semiconductor structures, which will result in the development of modularized, system-integrated and portable components for quantum repeaters. The Federal Ministry of Education and Research (BMBF) is funding the project with about 35 million euros over the next three years. The Institute for Nanostructure Technology and Analytics (INA) of the University of Kassel is involved with two working groups of Priv.-Doz. Dr. Mohamed Benyoucef (Nano Optics Group) and apl. Prof. Dr. Cyril Popov (Nano Diamond Group).

Due to the low interaction with the environment, photons are ideally suited to transport quantum information over long-distances. For long-haul quantum communication, the generation of quantum light states at 1.55 µm (telecom c-band) is of particular interest to establish low-loss quantum links in optical networks for secure data transmission due to the lowest attenuation losses in silica fibers at this wavelength. InP-based single quantum dots (QDs) are one of the possible candidates to reach the telecom c-band window. Semiconductor QDs can be miniaturized and manufactured in an integrated manner on semiconductor chips. This means that a large number of parallel semiconductor systems can be operated on one chip. The goal of the subproject “Telecom wavelength photonic structures” of the Nano Optics Group led by Priv.-Doz. Dr. M. Benyoucef is the realization of bright single QDs that emit single-photons and entangled photon pairs at telecom-C-band. In particular, the project will focus on in-situ control and optimization of the optical and structural properties of single QDs via epitaxial growth as well as the integration of quantum emitters in more complex photonic structures and pin/Schottky diode structures for spin manipulation. The work will be performed in close collaboration with many project partners from Germany such as: Characterization of the photon entanglement: TU Berlin, HU Berlin, TU Munich, and Uni Stuttgart. On-chip fibrer-coupling: TU Berlin and Uni. Stuttgart. Coherence properties of the photonic structures: TU Berlin and TU Munich. Theoretical investigations: Uni. Bremen. Spin manipulation: TU Munich and TU Dortmund.

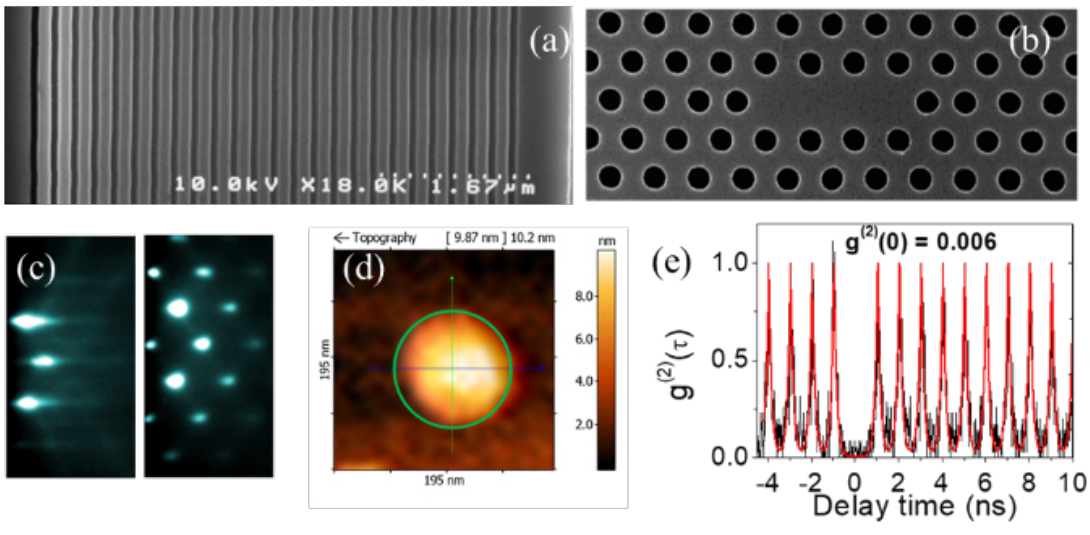

Fig. 1: (a) Scanning Electron Microscope (SEM) image of a grown DBR. (b) SEM image of L3 photonic crystals. (c) RHEED patterns: QDs formation (d) Atomic force microscopy image of single QD.(e) Single-photon emission at telecom wavelengths from single InP-based QDs.

Color centers in diamond have the advantages of long quantum coherence times of electron and nuclear spins in combination with efficient optical transitions as an interface to photons for the transfer of quantum information. The interface to photons is ensured either by a combination of microwave and optical transitions (NV centers) or by purely optical spin control (SiV centers). Diamond as solid-state platform offers the advantage of integration „on-chip“ with photonic elements for the targeted enhancement of the spin-light interaction. The aim of the subproject of the Nano Diamond Group led by apl. Prof. Dr. C. Popov is the fabrication of diamond membranes and diamond photonic structures (such as photonic crystals) using reactive ion etching and electron beam lithography. These structures will be coupled with color centers to increase the photon collection efficiency and applied as components for realization of demonstrators of quantum repeater nodes and fragments by project partners.

Further information

Website: https://www.uni-kassel.de/forschung/ina/technische-physik/forschung/nano-optics/

Link to BMBF Project: https://www.forschung-it-sicherheit-kommunikationssysteme.de/projekte/qr.x

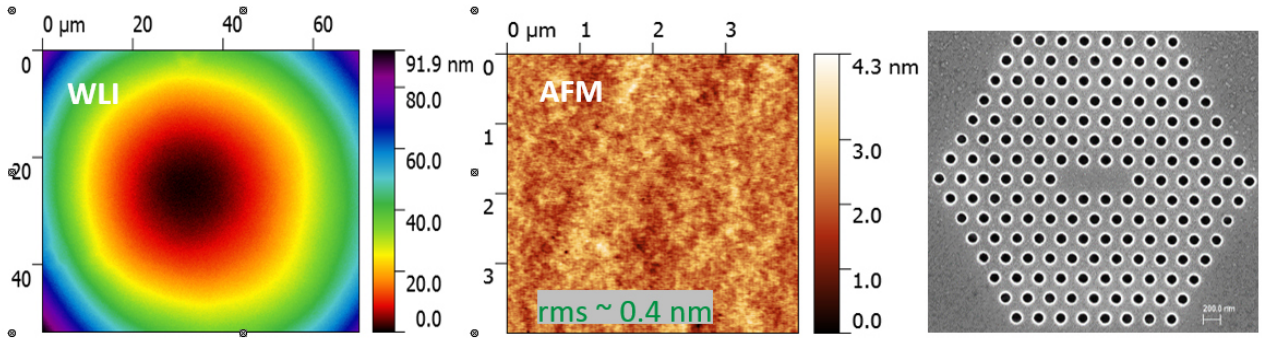

Fig.2 : (a) White Light Interferometer (WLI) image of a diamond membrane center, depicting the thickness variation. (b) Atomic Force Microscopy (AFM) image of 4 x 4 µm² membrane area featuring a low RMS roughness of 0.4 nm. (c) SEM image of a photonic crystal cavity (PhC) with a L3 cavity (air holes diameter 120 nm) inside a 600 nm thin single crystalline diamond (SCD) membrane.

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Modeling of electrical contact resistances at metal-plastic interfaces

An important aspect for the use of electrically conductive modified plastics is their contacting. In addition to methods that establish a contact subsequently, there are also numerous process-integrated solutions. Assembly injection molding is particularly worthy of mention here as a widespread contact-integrating plastics processing method. These contacting processes lead to a specific state of the interface transition between metal and plastic and of the plastic boundary layers, which can be described by local parameters of the two contact materials.

The aim of the DFG-funded project is the development of a model, which describes the electrical contact resistance at the interface between electrically conductive modified plastics and metallic contacts, as a function of the parameters of the interface transition, the plastic edge layers and the metal contact pin properties (Fig. 1, (a)). Furthermore, the model is to be quantified in order to be able to predict the contact resistance as a function of material parameters as well as processing variables in a context of realistic manufacturing processes.

Standard contact models (e.g. a-spot models) are of limited use to describe this interface electrically due to anisotropic properties of filled conductive compounds. The contact resistance depends not solely on the specific resistances of the used materials but also on the filler orientation at the contact area, the position and the connection to the conductive network. These are some local parameters with a critical impact on the contact resistance of such an interface. In turn, theses local parameters are directly depending on material properties (filler size, concentration, distribution etc.) and processing parameters (temperature, pressure etc.). In order to provide a basis for modeling electrical contact mechanisms in this specific case, the local contact resistance of the interface has to be determined.

One way of modifying polymer compounds to achieve conductivity is to utilize carbon-based fillers. Fig. 1 (b) shows a cryo-fractured contact area with carbon fibers in the polymer matrix. Such fibers have a diameter of about 7 µm and an average fiber length of 6 mm. Due to this high aspect ratio, high electrical conductivities can be achieved with relatively low filler contents. In addition, extremely fine conductive carbon blacks are to be used in this project, which have an average particle size of about 20 to 50 nm and form conductive paths through the formation of agglomerates.

To illustrate the general approach, a specimen consisting of a 30 wt% carbon fiber filled polypropylene compound (PPCF30) and seven contacts, overmolded via injection molding process is considered. Six of these contacts are arranged equidistantly around a central pin, which allows a symmetrical current flow for electrical characterization around the center contact as shown in the following electrical FEM simulation example. Results from filling studies of injection molding simulations allow the evaluation of the fiber orientations near the contact surface. These orientation tensors can serve as input for electrical FEM simulation of the near-contact compound and the compound volume in general. Here they are used for an assumption of the resulting contact resistances. The compound volume is initially considered to be homogeneously conductive.

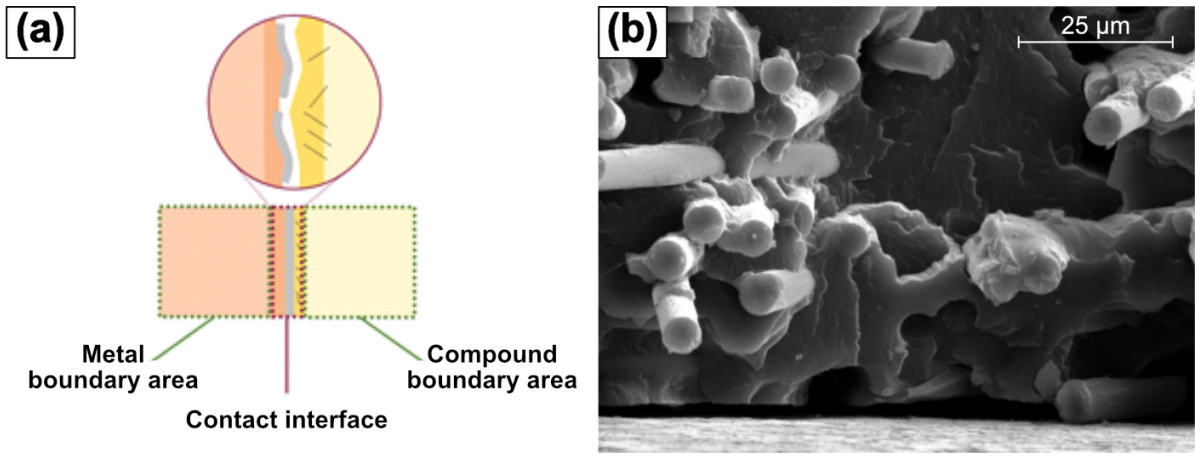

Fig. 1: Schematic overview of the boundary areas and the contact interface (a); Scanning electron microscope image of a cryo-fractured carbon fiber compound with an overmolded contact pin in the lower area (b)

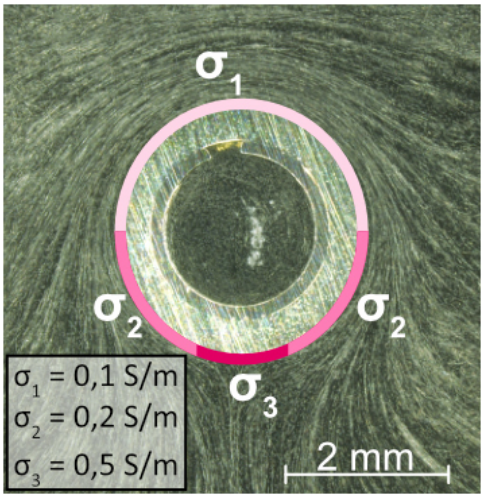

Fig. 2: Reflected light micrographs of PPCF30 samples with integrated central contact pin and proposed contact conductivities (assumption for FEM simulation)

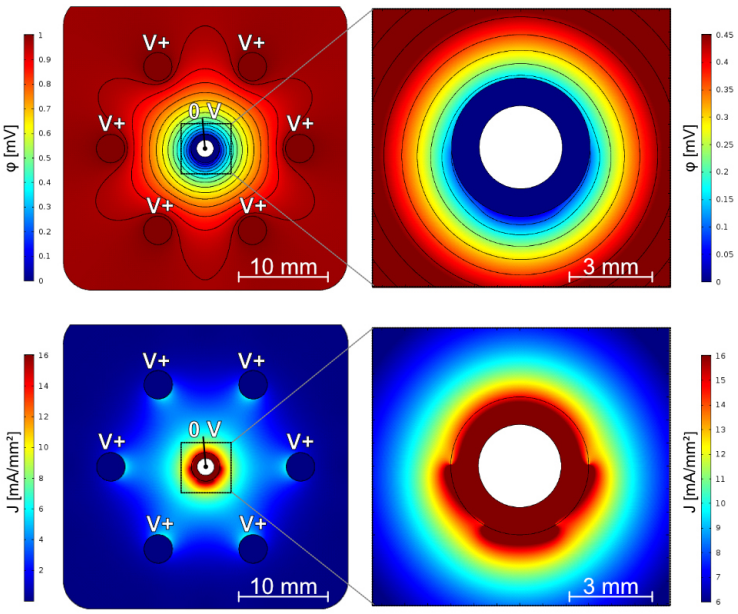

Fig. 3: Results of the FEM simulation of the electrical potentials (upper) and current density distribution (lower) at the specimen surface near the central contact pin. The applied voltages are labeled at the contact pins (+1 V).

Furthermore, imaging methods like reflected light microscopy (Fig. 2) or X-ray microtomography provide information about the local parameters. The fiber orientation can also be identified using microscopic images in comparison to simulated results. For illustration purposes, the contact boundary will be divided into three areas in a simplified manner. These three areas were determined and set based on results of previous research, as it is known that the formation of weld lines increase fiber concentration locally and therefore decrease the resistance in contact areas (area σ_3).

If these divided contact resistances are evaluated in an electrical FEM simulation with the assumed applied voltages, the results for the potential and the current density distribution are obtained as shown in Fig. 3. Different conductivities around the central contact are resulting in measureable potential differences. These results can be used to further derive the current density and finally under specific boundary conditions, to determine local resistances of this contact area.

Further information

Joining of Contact Pins and Conductive Compounds via Injection Molding – Influence of the Flow Situation on the Electrical Contact Resistance; H.-P. Heim, F. Mieth, A. Schlink, K. Wiegel und L. Brabetz, International Polymer Processing (2020), https://doi.org/10.3139/217.3879

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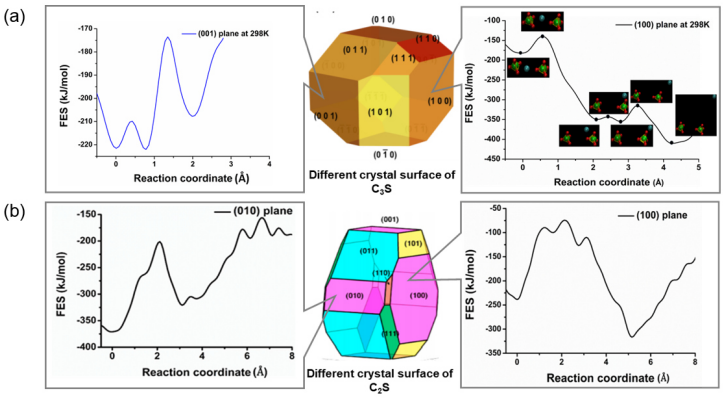
Elucidation of initial cement dissolution mechanism by the gap-bridging multiscale modeling approach (CEM-bridge)

Concrete is the most used man-made construction material in the world because of its flexibility and low production cost in comparison to other building materials. The global production of this irreplaceable material is approx. one ton per person per year. The main disadvantage is its enormous environmental CO_2 footprint. Producing cement clinker not only requires high amounts of energy, but it also releases approx. 5% of the global anthropogenic CO_2 and retreats 1.7% of total global freshwater. Complying with future climate regulations asked for a massive reduction of the cement clinker content, leading to the so-called eco-concretes. Understanding the reactivity of the remaining clinker content in eco-cements should help to improve the hydration performance of these classes of climate-friendly concretes. Advanced modeling will strongly support this development whenever starting from the fundamental nano-scale level. However, the molecular processes that underlay a cement–water reaction are still not fully understood, represented by a simultaneous interplay of various hydration mechanism stages like cement dissolution and precipitation of calcium−silicate−hydrates (C-S-H), forming the main binding phases of concrete. Therefore, a thorough understanding of the fundamentals that drive the dissolution processes of cement is of vital importance for the further development of environment-friendly-cements.

The main objective of this project is to develop an elementary physical/chemical bridging model for the initial dissolution mechanism of alite (C_3S, Ca_3SiO_5) and belite (C_2S, Ca_2SiO_4) cement clinker hydration that connects the nanoscale to the upscaled microscale level. Our previous study reviled that as (100) surfaces of C_3S dissolution being reactive and thermodynamically favorable toward hydration at 298 K (Fig.1a).



Besides, they also have indicated the air void formation as a result of their strong interaction with water, which initiates the capillary pore formation. Moreover, the water tessellation was a reason for the lower reactivity of (001) surfaces of C_3S during hydration. Additionally, among the surfaces of C_2S (100) is found reactive (Fig.1b). However, the reactivity is comparatively lower than the C_3S surfaces due to its compact crystal structure and absence of free oxygen. Therefore, no air void was observed after 600 picoseconds of hydration. In contrast, (010) was less reactive.

The approach starts with an in-depth understanding of alite and belite clinker surfaces by atomistic modelling of the surface complexation and far-from-equilibrium dissolution while differentiating between the various crystal planes. The upscaled model will quantify and validate the net dissolution rates, as an essential process which, later has to be considered by models attempting to capture the kinetics of cement hydration. The multiscale model will enable a deeper understanding of the alite and belite reactivity by predicting the dissolution rate as a function of the interplay between the mineral crystal structure and the chemistry of the surrounding solution. This understanding will allow new optimization routes for cement and cement replacing phases whose sustainability potential is directly impeded by their low reactivity. The sustainability of cementitious binders can be enhanced by the reduction of the clinker content without loss of hydration performance.

To achieve the main objective, a multiscale model will be developed at different scales by the two groups of the University of Kassel (UniKs) and the Technical University of Darmstadt (TUDa). UniKs will couple a biased molecular dynamics (MetaD) model with a reactive force field (ReaxFF) to obtain reaction paths and activation energies. The calculated rate constant of all atomistic reaction steps will be provided to TUDa group for developing the upscaled model using a kinetic Monte Carlo (kMC)

Fig. 1: Representative snapshot of dissolution mechanism (free energy profile) of Ca (a) from (100) and (001) surfaces of Alite, C_3S. (b) from (100) and (010) surfaces of Belite, C_2S RT (298 K).

method. In the project, the following stages will be considered, representing the sub-objectives: a) Evaluating the reactivity of different crystal planes of alite and belite; b) Obtaining atomistic reaction paths and activation energies for far-from-equilibrium solutions; c) Upscaling the atomistic rates of alite and belite dissolution, employing a kinetic Monte Carlo (kMC) approach; d) Investigating the effect of higher saturations in the surrounding solution on kMC results e) validation c) and d) by literature experimental data. First, the kMC upscaling dissolution rates will be validated on far-from-equilibrium conditions. This is of major importance, as it will enable a separation of the individual contributions of the combined dissolution-precipitation reaction processes for a better prediction and interpretation of the experimental research. Next, validation of kMC predictions with experimental results will consider the effect of higher saturation of the surrounding solution, to gradually approach realistic conditions for the initial cement hydration process (Fig. 2). The dissolution of alite/belite crystals is challenging as it is concurrently affected by the surface properties, presence of impurities and defects, and the chemistry of the surrounding solution. Therefore, the proposed CEM-bridge modelling approach will lead us to explore the dissolution mechanism of cement clinkers from atomistic scale to microscopic scale, which will be considered to be the major importance for the less reactive belite crystal for the further development of eco-cements.

Fig. 2: Interaction between the scales is based on the transition state theory (TST) to calculate the individual rates of the atomistic metaD simulations which are feeded to run the kMC simulations to obtain the mesoscopic dissolution rate. The kMC output on upscaled morphology and reaction rates are compared with experimental results.

Further information

[1] Salah Uddin, K. M. (2020) 'Elucidation of Chemical Reaction Pathways in Cementitious Materials' (Doctoral dissertation) Faculty of Civil and Environmental Engineering, University of Kassel. https://doi:10.17170/kobra-202009211835

[2] Salah Uddin, K. M.; Middendorf, B. (2019), Reactivity of different crystalline surfaces of C3S during early hydration by the atomistic approach, Materials 2019, 12(9), 1514; https://doi.org/10.3390/ma12091514

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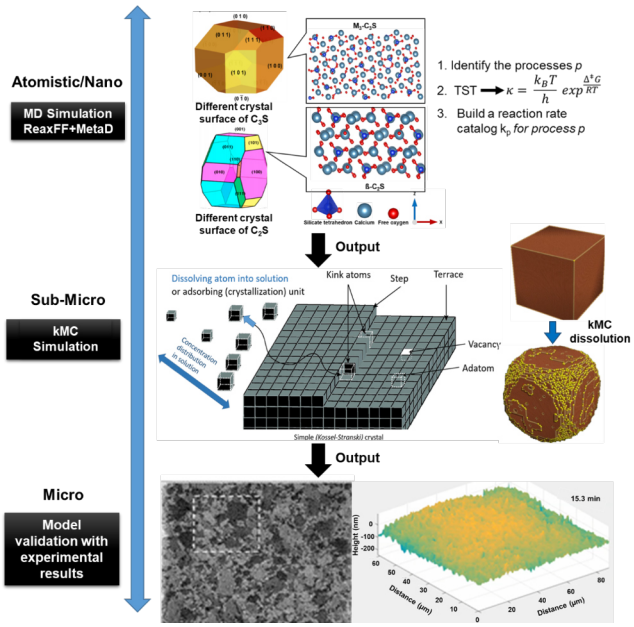

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Research Groups

Technological Physics Group - Faculty 10

The Technological Physics (TP) consists of four sub-groups with the following sub-topics:

Nano Optics, Nano Materials, Nano Fabrication & Devices and Nano Diamond.

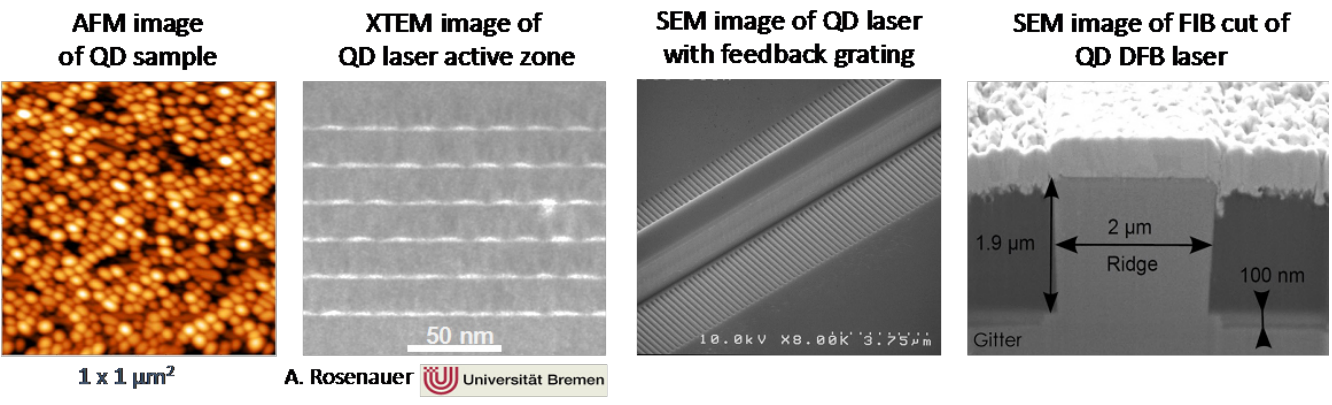
Two of them are headed by further CINSaT members, i.e., Mohamed Benyoucef (Nano Optics) and Cyril Popov (Nano Diamond). They introduced themselves in the Newsletter 1/2018, page 19 and 1/2017, page 21, respectively. Therefore, in this overview, the activities of the two remaining groups are highlighted.

The group operates also together with the Technological Electronics (TE) group of CINSaT member Hartmut Hillmer the Institute of Nanostructure Technologies and Analytics (INA). The general focus of TP is to realize and investigate semiconductor nanostructures and related nanoscopic materials as well as to apply them for new photonic or optoelectronic structures and devices. This includes fundamental research on, e.g., new materials, quantum physical phenomena and quantum optics and rather applied research, such as optoelectronic components and integrated circuits for high capacitance optical fiber communication networks and sensing applications. Two more PIs, apl. Prof. Dr. Cyril Popov heading the diamond group and PD Dr. Mohamed Benyoucef leading the nano optics group and, are also CINSaT members. More details on their topics are given in newsletters 1/2017 (p. 21) and 1/2018 (p. 19), respectively. The Technological physics group is also coordinating the LOEWE project SMolBits dealing with a new approach for future potential quantum computing based on molecular quantum bits and a nanophotonic solid state platform.

In figure 1, some images are shown made by an atomic force microscope (AFM), a transmission electron microscope (TEM) and secondary electron microscope (SEM) of semiconductor quantum dot materials and a laser with a distributed feedback (DFB) grating. The cross section of the device was prepared by focused ion beam (FB) milling on a finalized laser diode. These devices show ultra-narrow linewidth and high temperature stability related to quantum phenomena of the nanoscale material.

To improve the capability of the interaction with external partners in particular in the field of group III/V materials integrated on Si, a new epitaxial system, financed by DFG and the University (ca. 1.8 Mio € investment) could be recently installed (see figure 2), which allow now direct cooperations with silicon electronics foundries and research institutes by handling 8-inch Si wafers. This type of equipment is unique for any semiconductor research lab working on group III/V compounds, while typical GaAs and InP wafers have only diameters between 2 - 4 inch. These new capabilities may push the introduction of nanoscaled active materials in highly integrated optoelectronic circuits (OEICs). Several projects are already running, and further research applications are in preparation.

Fig. 1: Images of QD material and QD lasers. From left to right: (a) AFM image of InAs QDs grown on a semiconductor surface; (b) cross section TEM of the active zone of a laser with 6 QD layers separated by 20 nm thick barriers; (c) SEM image of a first order grating of a QD DFB laser; (d) crosscut perpendicular to the waveguide of a fully processed QD laser performed by FIB. The depth of the grating trenches of 100 nm is indicated.



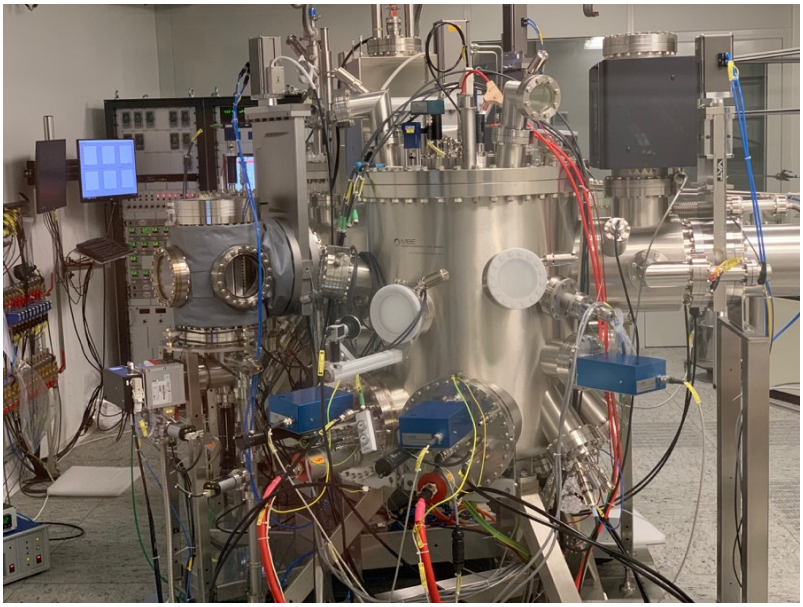


Fig. 2: Dual-chamber epitaxial system with a Si/Ge and a group III/V chamber installed in the clean room of INA. The system can handle multiple 2 and 3 inch as well as single wafers up to 8 inch in diameter.

Fig. 3: Group picture at internal group seminar in the State Domain Frankenhausen, September 2020. Large spacing was needed due to the COVID-19 safety rules.

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Latest Reports

CINSaT autumn colloquium

First CINSaT Autumn Colloquium in presence form since 2019 attracts many professors, academic staff, and student to the lecture hall.

On Wednesday, 3rd of November 2021, the annual autumn colloquium of the CINSaT took place in lecture hall 282 at the Campus Heinrich-Plett-Straße of the University of Kassel. Numerous professors, doctoral students, as well as undergraduate and graduate students from various disciplines waited excitedly for the lectures of the speakers. The autumn colloquium, which is open to all who are interested, offers not only the opportunity to listen to interesting topics on current research, but also to inform themselves about the current research contents of the CINSaT during the poster session. After being held in virtual form in 2020, this year's colloquium was held in presence again. Of course, this required some adjustments to meet the hygiene rules of the University of Kassel. Face masks were mandatory for the whole duration of the colloquium and the whole venue was stretched out in the foyer of the AVZ to accommodate over 100 participants of the event. Only fully vaccinated, recovered, or currently tested persons were allowed to participate, and the contact information were collected.

The colloquium started with a welcome speech of Prof. Dr. Johann Peter Reithmaier, head of the CINSaT, who led into the first part of the lecture series that was opened by Prof. Dr. Thomas Weitz from the University of Göttingen with his talk about "Quantum transport in organic semiconductors and bilayer graphene at the nanoscale". This interesting talk by our guest was followed by a talk titled "Exploiting light-molecule interaction: From non-linear optics to chiral matter-wave" from Dr. Daqing Wang of the Light-Matter-Interactions Group (Prof. Dr. Kilian Singer), which was also his application presentation for an associated CINSaT membership. After a half-hour coffee break with cookies and cake, which was used not only to get to know each other, but also for the first review of the posters, the second part of the lecture series followed. CINSaT member Prof. Dr. Hartmut Hillmer gave a talk about "Mysterious quantum-optic forces in the nano-cosmos" and afterwards the session was completed with a talk titled "Improved light sheet microscopy and the dynamic quantitative analysis of morphogenetic mechanisms in development biology" given by CINSaT member Prof. Dr. Arno Müller.

The poster session following the lectures showed 52 contributions from the groups of the CINSaT members. The foyer in front of lecture hall 282 offered not only enough space for the numerous poster contributions, but also for extensive scientific discussions and the exchange of information on current research content within the CINSaT. The catering of the Studentenwerk of the University of Kassel provided again for the well-being during the event. The conclusion of the event was the presentation of the

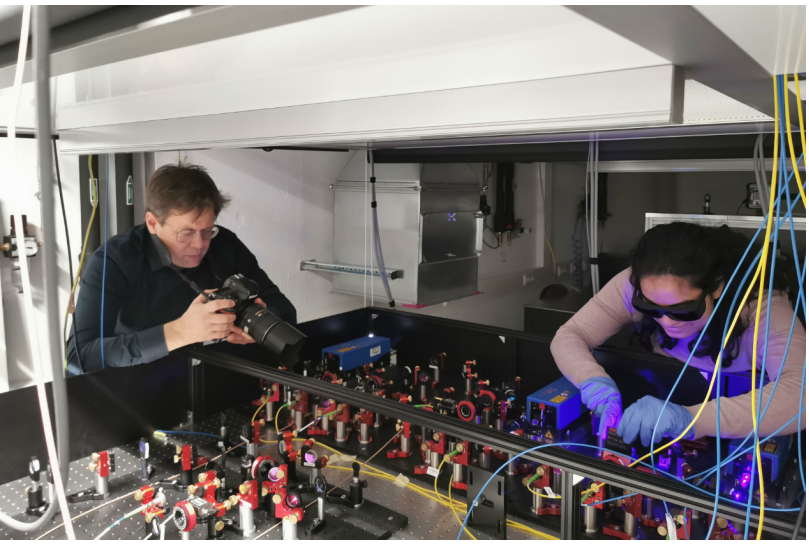
poster prizes awarded by this year's jury - consisting of CINSaT members Prof. Dr. Stefan Böhm, Prof. Dr. Philipp Demekhin, Prof. Dr. Friedrich Herberg and Prof. Dr. Rudolf Pietschnig - for the three best poster contributions was awarded (1st prize tablet, 2nd prize Raspberry PI starter kit, 3rd prize external SSD). The jury emphasized the high scientific quality of the posters.

This year, the first price was given to the poster "Deep subwavelength sensing in the THz regime with plasmonic bow-tie antennas on a silicon strip waveguide" by Soenke Grüssing from the Computational Electronics & Photonics Group (acting group leader Prof. Dr. Hartmut Hillmer). The second and third prize were given to Pascal Plettenberg (Condensed Matter Physics and Ultrafast Phenomena Group, Prof. Dr. M. Gacia) with his poster entitled "Machine-Learning interatomic potential for laser excited silicon" and Ly Nguyen (Biophysics Group, Prof. Dr. J. Kleinschmidt) for her presentation about “Interactions of BamD of the Barrel Assembly Machine (BAM) Complex with phospholipid Bilayers and BamA”, respectively. Due to the high number of participants, both in the audience as well as the poster contributions, and the thematically balanced lectures of the speakers, the CINSaT Autumn Colloquium was a success.

Shooting of the CINSaT films

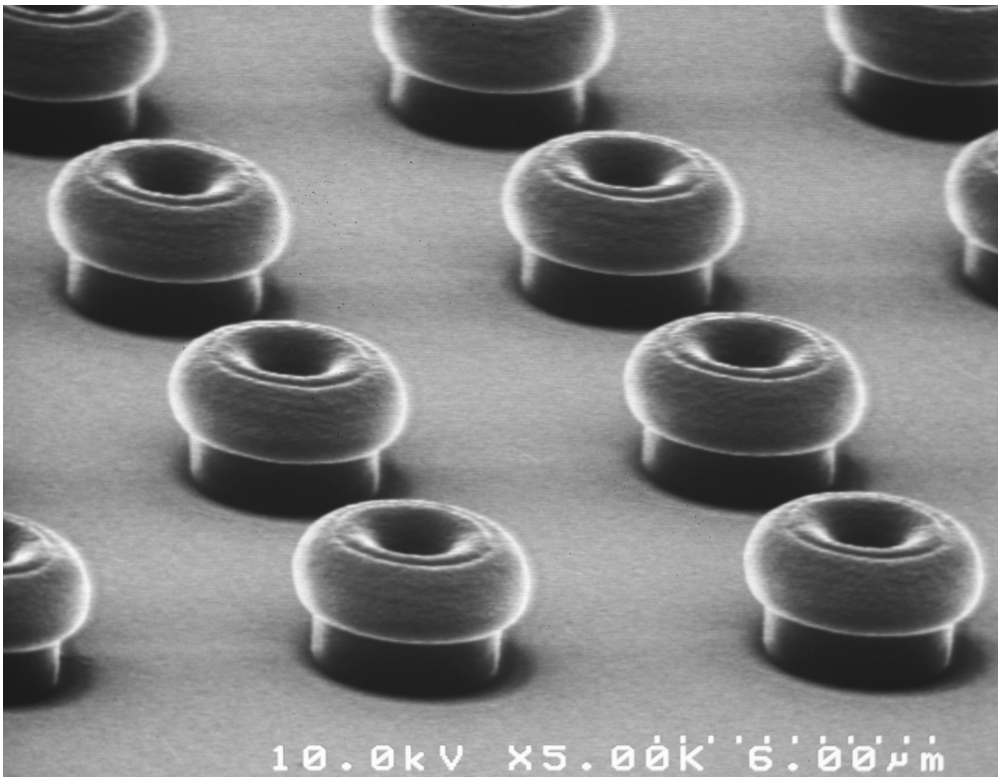
Between the 26th of October and 1st of November 2021 the shootings of the upcoming CINSaT films were carried out. The film crew consisted of Paavo Blåfield (photographer and owner of the executing studio), Paul Mayer (camera operator) and Tobias Böhm (sound technician). On five days the film crew visited the 23 participating CINSaT members spread over three different locations of the University of Kassel to film laboratories, devices, and record statements. Everyday thousands of images and several hours of film and sound recordings were produced. Over 50 people gave statements to explain their work or the devices they use.

In total seven films will be produced until the end of the year. One film about the CINSaT itself with around 180 seconds of runtime and six films about the individual focal points, each around 12 seconds runtime. The films aim to spark interest in the works of the CINSaT and its focal point and will be distributed with the social media channels of the University of Kassel to attract upcoming students as well as young scientific talents looking for a new challenge. The films are expected to be released in the beginning of next year.



Nano Arts

In this section, artistically appealing images from the CINSaT groups will be presented. If you obtain any kind of visually appealing and fascinating data during your experiments with focus on micro- and nanometer length scales, you are cordially invited to submit your contribution to the editors.



SEM micrograph of three-dimensionally curved toroidal magnetic thin film caps prepared by two-photon lithography and sputter deposition.
(Christian Janzen, Functional Thin Films and Physics with Synchrotron Radiation)

Photo: Campus Heinrich-Plett-Straße, Press and Public Relations Office University of Kassel, Studio Blåfield

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