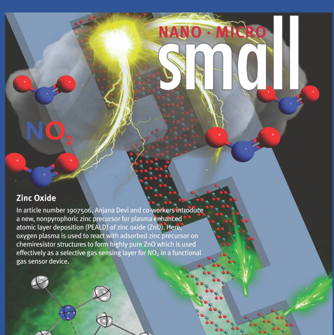
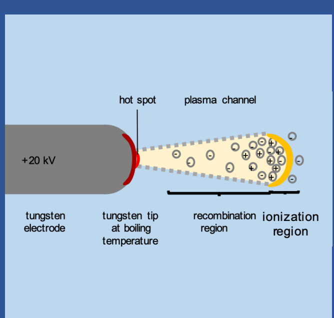
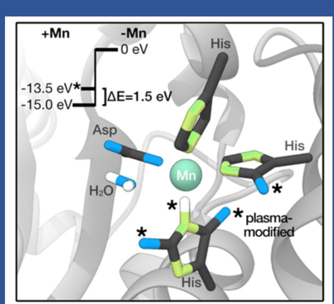
NEWSLETTER

IN THIS ISSUE

EDITION 10 — 2/2020







SFB-TR 87

SFB 1316 Transient Atmospheric Plasmas *from plasmas to liquids to solids*

Foreword to the 10th newsletter

We look back on a year in which many things have been reorganized and a leap towards digital and mobile modes of cooperation have been achieved. Certainly, the new way of working has advantages, nevertheless, important aspects in ones scientific everyday life have suffered. Therefore, we hope for a better year in 2021!

The scope and content of the newsletter keeps its normal focus even if external circumstances create difficult conditions. For example, the preparations for sending of the newsletter alone will not be done by several people in one room as usual, but one after the other.

Nevertheless, in the last half year a number of outstanding scientific findings could be produced, which is shown by the article below alone. Furthermore, many workshops were held digitally, which made it possible to increase the number of participants, as being documented on the next pages.

Last but not least, there were three personnel changes. First the CRC 1316 assistance, Verena Banach was recruited as a replacement. Also to be mentioned is the newly appointed Assistant Professor Judith Golda, who started her working group in November 2020. As successor of Peter Awakowicz, Thomas Mussenbrock will lead the AEPT chair in the future.

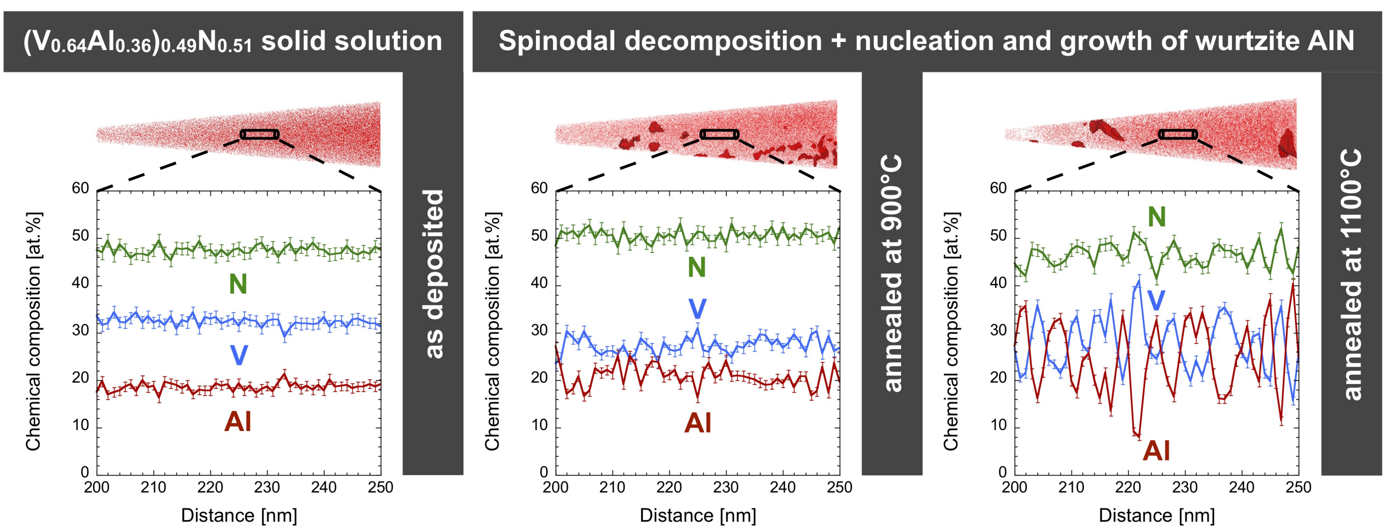
Marina Prenzel, public relations for the SFB-TR 87 and CRC1316

Honour of research publication

Paper from SFB-TR 87 among editor's choice of Surface and Coatings Technology

The Editors of Surface and Coatings Technology recently published an Editor's Choice selection of key papers that highlight some of the best current research published in the journal until June 2020. The article "Spinodal decomposition of reactively sputtered $(V_{0.64}Al_{0.36})_{0.49}N_{0.51}$ thin films" (doi: 10.1016/j.surfcoat.2020.125641) from project A3 is among this Editor's Choice selection, will be granted with promotional access for 12 months and is therefore freely available from July 2020 until June 2021.

Marcus Hans, project A3 of the SFB-TR 87

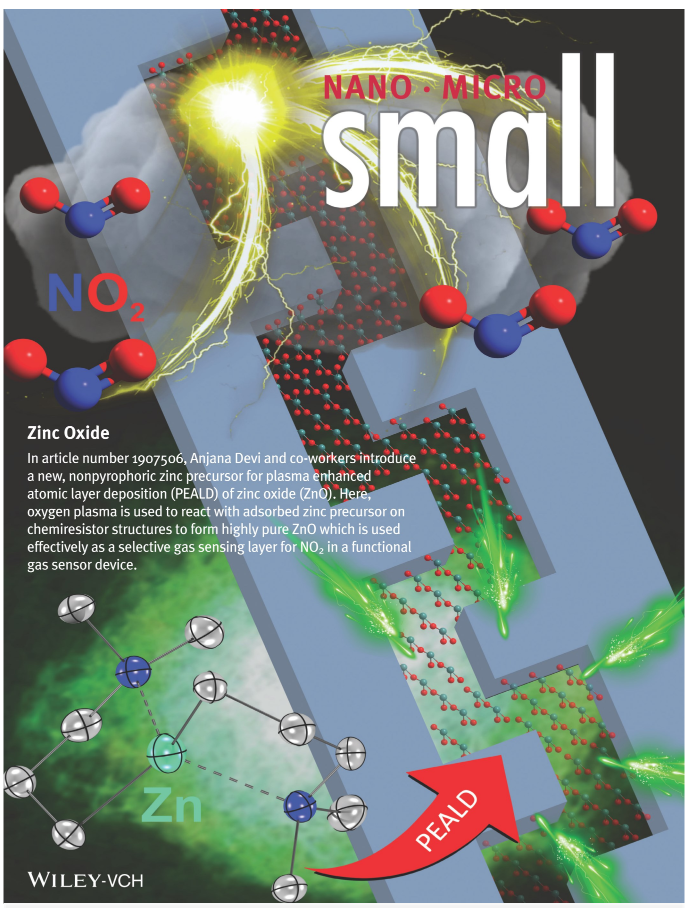


(Source: https://www.journals.elsevier.com/surface-and-coatings-technology/editors-choice/the-editors-of-surface-and-coatings-technology-are-delighted)

From precursor chemistry to gas sensors

In project B4 of the SFB-TR 87 Devi, a new atomic layer deposition (ALD) process for zinc oxide (ZnO) thin films was developed that utilizes a new and safe chemistry. For all ALD processes, metal-organic complexes, so-called precursors, are evaporated and pulsed into the reaction chamber. Here, the precursor reacts in two separated self-limiting reactions first, with the surface and second, with a co-reactant, in this case an oxygen plasma, to form a thin film. The two reactions are repeated in a cyclic manner and by adjusting the number of ALD cycles, the thin film thickness can be tuned with atomic precision over three-dimensional surface geometries. Typically, for the ALD of ZnO, the precursor diethyl zinc (DEZ) is used. However, this chemical is highly pyrophoric, i.e. ignites immediately upon contact with air, and is thermally unstable which requires stringent safety precautions and limits the deposition temperature as well. In this research work, that was recently published in small [1] as a result of a collaboration between the research groups of Prof. Devi and Prof. Awakowicz, a new non-pyrophoric precursor, called bis-(3-N,N-dimethylamino)propyl zinc (BDMPZ), that retains the advantages of DEZ in terms of high reactivity but possesses enhanced thermal stability at the same time. Thus, an ALD process could be developed that widens the deposition temperature range from 60°C to 160°C, thereby filling a deposition temperature gap for which no precursor was available. The resulting ZnO thin films are uniform, pure and pinhole-free, typical for ALD thin films and were therefore applied as gas barrier layer (GBL) and gas sensing layer to detect NO_2. It was shown that even a 7.5 nm thin film on polyethylene terephthalate (PET) substrate can sufficiently decrease the oxygen transmission rate (OTR) by 98.7% compared to a bare PET substrate. Additionally, the ZnO thin films are electrically conductive which was advantageous to build a gas sensor that shows an increasing resistivity when exposed to NO_2 at concentrations as low as 0.06 ppm without cross-sensitivities toward CO and NH_3. With these promising results, it was demonstrated, that the layers deposited using BDMPZ in ALD processes can already compete with the ZnO layers deposited from the commercially available DEZ precursors that is widely used in industry.

Lukas Mai and Anjana Devi demonstrating the described layers.



Cover page of the journal issue with the picture of the article from Mai et al.

[1] Small **16** (22), 2020. *1907506* (doi: 10.1002/smll.201907506)

Lukas Mai, project B4 of the SFB-TR 87

Engineering research group has a successor

Thomas Mussenbrock appointed at RUB

Since November 1, 2020, Prof. Dr.-Ing. Thomas Mussenbrock has held the chair of plasma technology in the Faculty of Electrical Engineering and Information Science.

He conducts research in the field of low temperature plasmas as well as on nanoelectronic and nanoionic devices. His team develops analytical and numerical methods for modeling and simulation and applies them in conjunction with experiments. "At the Ruhr-University Bochum, I find the ideal conditions for this," explains Thomas Mussenbrock. "Here, these experiments run right next door. I can follow them live and draw conclusions for our simulations, which in turn have a positive effect on the next experiments. In concrete terms, it is often a question of getting energy into a plasma efficiently and in a targeted manner. "Our goal is to excite only very specific particles." For Thomas Mussenbrock, much of his work deals with transport of energy and matter. "We are aiming to understand the macroscopic behaviour of the systems on the basis of the microscopic dynamics of the atoms, molecules, electrons and photons involved," the researcher explains.

More specifically, plasmas play a decisive role in the fabrication of microelectronic devices and circuits, for example. "More than 70 percent of all manufacturing steps are plasma-assisted," says Thomas Mussenbrock. "It is not for nothing that they say: No plasma, no iPad.

The chair of plasma technology is member of three collaborative research centres among others. This research centres are the collaborative research centre transregional SFB-TR87 "Pulsed High-Power Plasmas for the Synthesis of Nanostructured Functional Layers," the CRC 1316 "Transient Atmospheric Pressure Plasmas - from Plasma to Liquids to Solids," and the CRC 1461 “Neurotronics: Bio-inspired Information Pathways”.

adapted from Arne Dessaul, RUB

Change of staff

New administrative assistance for the CRC 1316

Since October of this year, Verena Banach is working as the assistant for the CRC 1316 and is responsible for the administrative work. Verena's responsibilities include financial tracking, quarterly calls of funds and distributing, planning project meetings or workshops as well as keeping the CRC 1316 website updated.

Please do not hesitate to contact Verena via mail (verena.banach@rub.de) or phone (0234-33-23672) if you have any queries or you may need assistance.

Ion collisions and heating in HiPIMS plasmas

One of the goals of the SFB TR 87 is to further our understanding of the physical process inside high power impulse magnetron sputtering (HiPIMS) plasmas. In such discharges, ions are attracted from the plasma towards a surface, the so-called target. The fast impact of ions removes atoms from this target surface, a process called sputtering, which then move through the discharge. Eventually, the sputtered atoms will reach a work piece and form a coating there. For the quality and the growth rate of these coatings, the particle transport through the discharge is of major importance.

of the sputtered particles become ionized. On the one hand, this means that these ions are affected by electric fields in the plasma, which will back attract them towards the target surface. This process has been attributed with limiting the deposition rate of HiPIMS discharges compared to traditional magnetron sputtering. On the other hand, however, ions have a much higher probability to collide with each other than neutrals. These so called Coulomb collisions were the focus of the recent publication.

> *"Our work shows that the ion movement in HiPIMS discharges is not only affected by strong electric fields, but also by a high amount of Coulomb collisions. Those collisions redistribute the initially directed movement of ions in velocity space and might contribute to the lower deposition rate commonly observed in HiPIMS plasmas."*

In a recent publication, the projects A5 and C7 investigated the transport of these sputtered particles more closely. In traditional magnetron sputtering, collisions are often assumed to play a minor role because of the low pressure inside the chamber during the deposition process. However, HiPIMS plasmas are operated at short high voltage pulses, with power densities that are orders of magnitude higher than traditional magnetron sputtering. Consequently, many

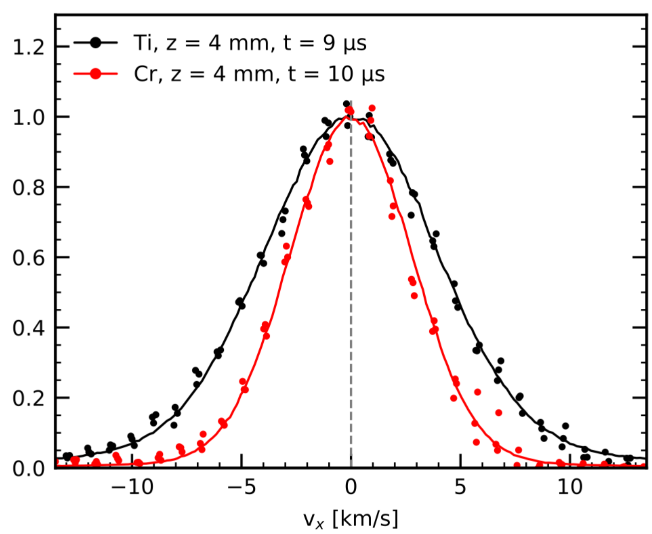


Figure 1: Velocity distribution function of chromium and titanium ions in the direction parallel to the target surface and at a target distance of 4 mm. Points indicate the OES measurements and lines show the result of the Monte-Carlo simulation.

The authors of A5 and C7 used optical emission spectroscopy to analyze the light emitted by the plasma during the deposition. The movement of particles causes a broadening of optical emission lines due to the Doppler effect. This was used to determine the velocity distribution function of chromium and titanium ions which allowed the authors to deduce the average energy and movement of these particles (see Fig. 1).

Surprisingly, the analysis revealed effective ion temperatures of up to 4.5 eV for chromium and 9 eV for titanium ions. In order to explain these extreme ion temperatures, the authors investigated the redistribution from the initial energy gained during the sputter process into a Maxwell distribution that is caused by the frequent ion-ion collisions. This energy redistribution was simulated using a Monte Carlo approach, which showed good agreement to the measured data. Since all of the observed energy of these ion species can be explained with this energy redistribution alone, Ohmic heating by the electric field seems to play only a minor role.

Summarizing, these findings show that HiPIMS plasmas are highly collisional. This also has implications on the deposition rate of such discharges, which is an important consideration for applications.

The publication is titled „Velocity distribution of metal ions in the target region of HiPIMS: the role of Coulomb collisions" and was recently published in Plasma Sources Sci. Technol. 29 (2020) 125003 (12pp).

Julian Held, project A5 of the SFB-TR 87

Unravelling ns plasma physics of streamers in water

The complex nature of nanosecond plasmas in liquids makes these discharges a great deal of attention nowadays. These discharges are an important method to trigger the water chemistry for electrolysis or for biomedical applications in plasma medicine. The understanding of these chemical processes relies on knowing the variation of the temperatures in these dynamic plasmas. This is analyzed by monitoring nanosecond pulsed plasmas that are generated by high voltages (HV) at 20 kV and pulse lengths of 15 ns applied to a tungsten tip with 50 micrometer diameter immersed in water. Plasma emission is analyzed by optical emission spectroscopy (OES) ranging from UV wavelengths of 250nm to visible wavelengths of 850nm at a high temporal resolution of 2 ns.

"Nanosecond plasmas discharges are an important method to trigger the water chemistry for electrolysis or for biomedical applications in plasma medicine."

The spectra are dominated by a black body continuum and line emissions from the hydrogen Balmer series. The continuum radiation originates from the hot tungsten surface, which acts as the powered electrode. Typical temperatures from 6,000K up to 8,000K are reached for the tungsten surface corresponding to the boiling temperature of tungsten at varying tungsten vapor pressures. The analysis of the ignition process and the concurrent spectral features indicate that the plasma is initiated by field ionization of water molecules at the electrode surface. At the end of the pulse, field emission of electrons can occur. During the plasma pulse, it is postulated that the plasma contracts locally at the electrode surface forming a hot spot. This causes a characteristic contribution to the continuum emission at small wavelengths. The spectra also show pronounced emission lines of the hydrogen Balmer series.

The data indicate two contributions of the hydrogen line radiation that differ with respect to the degree of self-absorption. It is postulated that one contribution originates from a recombination region showing strong self-absorption and one contribution from an ionization region showing very little self-absorption. The emission lines from the ionization region are evaluated assuming Stark broadening, that yielded electron densities up to 5×10^{25} m^{-3}. The electron density evolution follows the same trend as the temporal evolution of the voltage applied to the tungsten tip. The propagation mechanism of the plasma is similar to that of a positive streamer in the gas phase, although in the liquid phase field effects such as electron transport by tunnelling should play an important role.

It is striking that the electron density follows closely the voltage applied to the electrode during the rising and falling edge of the pulse. In nanosecond plasmas in gases at atmospheric pressures, the voltage and current exhibit usually a delay in between with the voltage rising first followed by the current due to the delayed build-up of the electron density in the ionization avalanche. During the plasma propagation in the liquid,

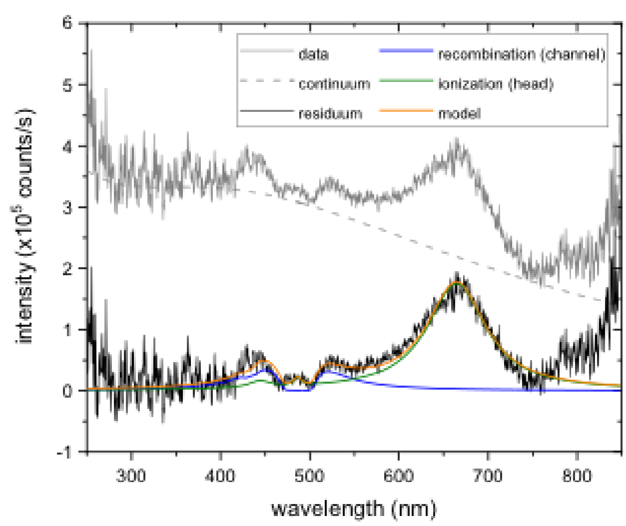


Figure 1: Emission spectrum at 12 ns after ignition (solid gray line), continuum radiation from black body radiation and hots spot emission (dashed gray line) and resulting residuum (solid black line). The latter is fitted with a model (orange) including an ionization zone at the streamer head (green line) and a recombination zone within the plasma channel (blue).

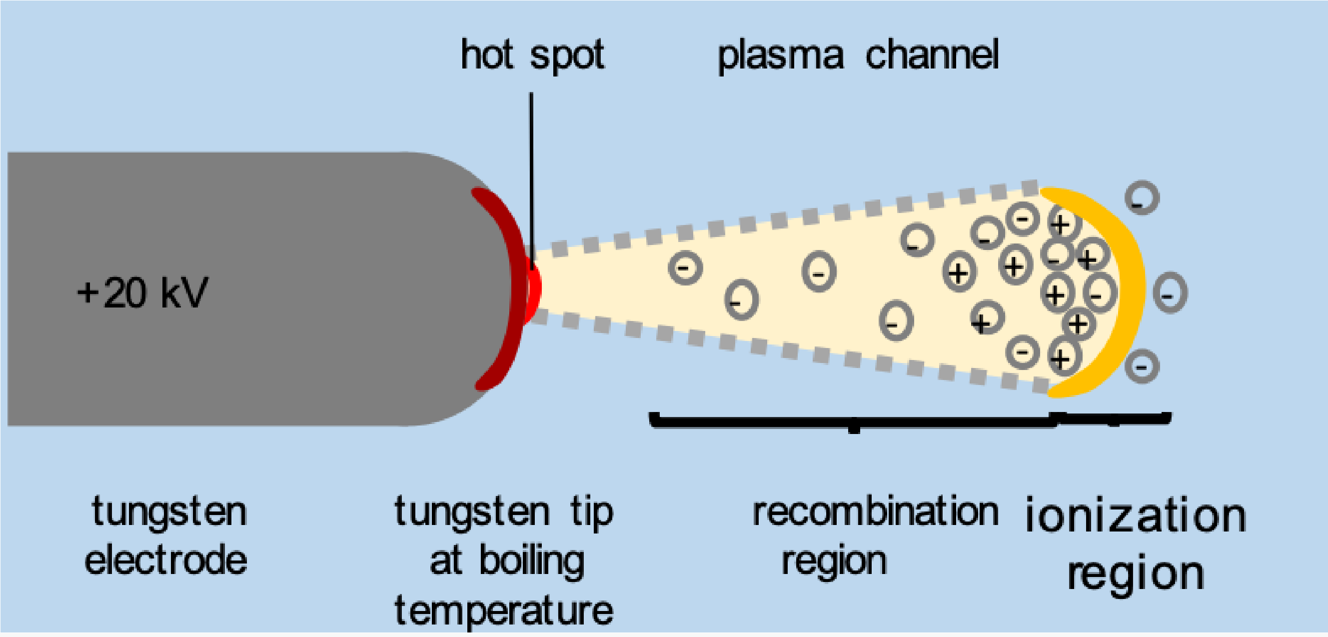


Figure 2: Sketch of streamer propagation inside the liquid illustrating different origins of emission.

however, the density of species is three orders of magnitudes higher, so that the build-up of charges is expected to be much faster compared to the variation of the voltage. The same also holds for recombination that should exhibit time constants of the order of ps at these densities. The actual electron density is then a balance between generation of free electrons in the high electric fields and their loss due to recombination. This is consistent with the observation that the electron density also follows the decrease of the voltage with a time constant of 8 ns. The decay of the electron density is not a free decay due to recombination, but rather follows a decreasing equilibrium value as a competition between ionization and recombination.

[1] K Grosse et al 2020 *Plasma Sources Sci. Technol.* **29,** 095008, doi: 10.1088/1361-6595/aba487

[2] A von Keudell et al 2020 *Plasma Sources Sci. Technol.* **29,** 085021, doi: 10.1088/1361-6595/aba4b9

Katharina Grosse, project B7 of the CRC 1316

Workgroup IANiS

Hands-on Workshop 03 — „Machine Learning for Materials Science and Plasma Science“

Data acquisition and analysis is of crucial importance for all scientific projects of the SFB-TR 87. This holds for project conduction experiments in the laboratories and theoretical projects the like. It is of particular relevance for the correlation approach pursued within the plasma surface model for the global plasma parameters during thin film deposition and the corresponding coating properties. To support this initiative, the topic of “Machine Learning for Materials Science and Plasma Science” was addressed in an hands-on workshop of the working group IANiS on August 4th. Due to the Covid-19 pandemic, this workshop with participants from all four universities collaborating within the SFB-TR 87 was conducted virtually. The workshop started with a brief introduction to the exemplary data used in the workshop – ICCD camera images of plasma spoke patterns obtained with different HiPIMS plasmas conditions. Following a brief introduction to data clustering methods, the participants were able to gain first-hand experience by applying different clustering techniques in small interactive groups. In a number of alternating sessions of data science foundations (e.g., classification tasks, generative methods) and corresponding hands-on experiences, the workshop again fostered the interdisciplinary exchange between PhD students and postdocs and therewith contributed to the success of SFB-TR 87.

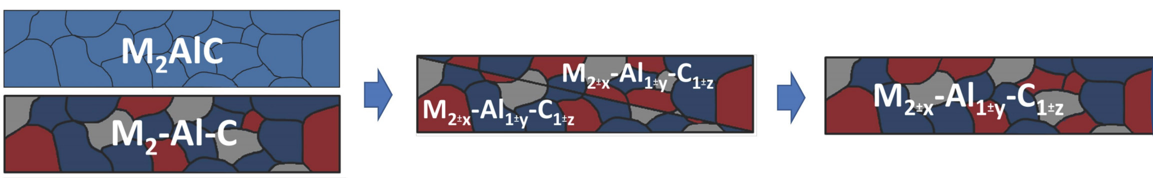
Lars Banko, Marcus Hans & Jan Trieschmann, SFB-TR 87

Effect of target peak power density on composition of sputtered thin films from composite/compound targets

The aim of transfer project T1 is the knowledge-based design of composite/compound sputter targets for the synthesis of stoichiometric thin films by using HPPMS. Composite/compound targets are beneficial with respect to reproducibility and process stability for industrial thin film growth applications since homogeneous coatings have to be formed over large areas on a multitude of substrates. However, it has been shown that the chemical composition of thin films sputtered from a Cr-Al-C composite target exhibited substantial aluminum depletion as a function of the applied target peak power density in combination with substrate bias potential as well as growth temperature [1,2]. Within this project the effect of industrially-relevant deposition parameters (target peak power density, substrate bias, growth temperature and substrate rotation) on the composition of MAX phases sputtered from M-Al-C composite/compound targets is investigated. MAX phases are interesting for industrial applications due to combination of ceramic and metallic properties and the use of Cr-Al-C, Zr-Al-C as well as Hf-Al-C targets enables a systematic comparison of MAX phase thin films with significant mass differences.

Since the project T1 relies on high-quality, industrial-sized sputter targets and generates understanding of target design criteria for specific industrial deposition conditions, this project was proposed jointly with Plansee Composite Materials GmbH. The R&D scientists at Plansee are not only experts in target manufacturing utilizing technologies such as pressing, forging, hot pressing as well as spark plasma sintering, they have also developed expertise and the necessary processing tools to produce targets with 'off-stoichiometric' compositions. While the project aims at the growth of stoichiometric MAX phase thin films, the targets are not produced from MAX phase raw material and desired compositions are realized by mixing metals as well as carbide phases. The discrepancies between target and film composition are evaluated in a first step by using stoichiometric composite/compound targets. Based on these findings, split targets with varying composition are designed in close collaboration with the application partner, enabling the growth of M-Al-C thin films with a chemical composition spread along the target length. Thereby, the required target composition for the growth of stoichiometric MAX phase films will be identified for different combinations of target peak power density, substrate bias, substrate temperature and substrate rotation. The here obtained understanding allows for knowledge-based design of composite/compound target compositions which result in stoichiometric MAX phase thin films. Transfer project T1 benefits from and contributes to the plasma surface model of SFB-TR 87.

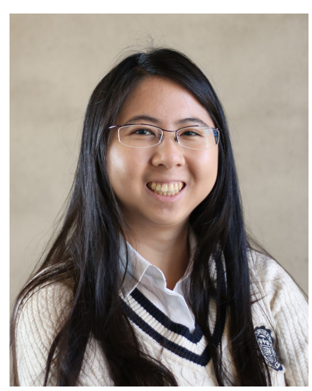
Knowledge-based target design for synthesis of stoichiometric MAX phases utilizing HPPMS



[1] H. Rueß, M. to Baben, S. Mráz, L. Shang, P. Polcik, S. Kolozsvári, M. Hans, D. Primetzhofer, J. M. Schneider, Vacuum 145 (2017) 285-289, https://doi.org/10.1016/j.vacuum.2017.08.048.

[2] H. Rueß, J. Werner, Y. Unutulmazsoy, J. W. Gerlach, X. Chen, B. Stelzer, D. Music, S. Kolozsvári, P. Polcik, T. E. Weirich, J. M. Schneider, Journal of the European Ceramic Society, accepted https://doi.org/10.1016/j.jeurceramsoc.2020.10.072.

Yu-Ping Chien, project T1 of the SFB-TR 87



Gas barrier coatings for returnable PET bottles

HMDSO based silicon oxide coatings are a standard application for PET bottles in the packaging industry. Up to now, applicability of these coatings is limited to single use PET bottles. With regard to resource efficiency and reduction of plastic waste, enabling the use of this technology for returnable bottles is not only of commercial interest, but also concerning environmental protection and ecology. Together with their industrial partner KHS Corpoplast GmbH, the research teams of RWTH Aachen and Ruhr-Universität Bochum deal with this topic. The main issue regarding silicon oxide based coatings on returnable bottles is the washing process: After return, bottles are washed with a NaOH solution to ensure a clean and safe packaging for the following refilling with beverages. The lye corrodes oxide coating as well as the underlying PET substrate. As a result, the coating loses its barrier property and the PET surface is chemically and morphologically altered, which prohibits a simple recoating. Therefore, the development of lye resistance is a key issue. In a first step, coating resistance against NaOH lye was qualitatively assessed by taking advantage of the reaction between aluminium and NaOH lye to hydrated sodium aluminate and hydrogen:

$2\,Al + 2\,NaOH + 6\,H_2O$ à $2\,NaAl(OH)_4 + 3\,H_2$

Hydrogen formation can be seen with a microscope as bubbles on the observed sample. This happens immediately when NaOH lye is trickled on uncoated Aluminium. On a coated sample, time until bubble formation serves as a means to evaluate the coating's resistance against the lye.

This way, low pulse power and short pulses of pure monomer gases were identified for optimal resistance coatings. These findings could be confirmed by electrochemical impedance spectroscopy and cyclic voltammetry. Additionally, these methods revealed that coatings with better resistance exhibit lower porosity. AFM scans revealed that with lower roughness, a better resistance was observed. Concerning chemical composition of lye resistant coatings, XPS and FTIR were conducted. High resistance coatings show high carbon content and a higher content of methyl groups and Si-O-Si-bonds.

In summary, these results suggest that low fragmentation of the monomer during film deposition seems to promote the lye resistance of the coating. It can be concluded that a high amount of methyl groups in these films provide stability against chemical attacks due to steric shielding.

These findings have already been validated in conditions similar to commercial application. A HMDSO based SiO_x barrier layer was deposited on PET foil. Subsequently, a top layer for lye resistance was deposited on the barrier layer. The industrial washing process was simulated by an exposure to NaOH solution at 57°C for 10 min for several times. As a benchmark for coating conditions, the oxygen transmission rate (OTR) was measured initially and after every exposure to the NaOH solution. Nearly no rise in OTR can be seen up to nine exposures. The OTR rises steadily with every NaOH exposure.

These promising results were successfully transferred to an industrial machine for the coating of PET bottles. In Figure 1, the results of a 12 day exposure to NaOH at 57°C is shown. While the uncoated bottle is visually corroded by the lye (left); the bottle with a corrosion resistant coating (middle) is optically unaffected compared to a new bottle (right).

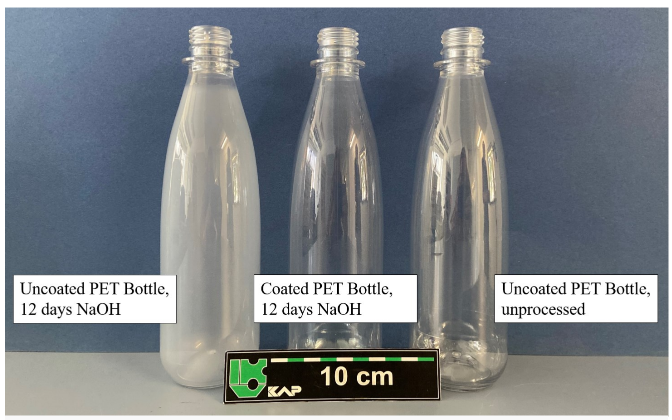


Figure 1: Long duration NaOH exposure experiment

The next step is the process characterisation based on plasma parameters, like electron temperature and density during deposition processes on the different coating setups. Here, different approaches on plasma diagnostics are pursued with focus on optical emission spectroscopy in combination with a collisional radiative model. This way, the influence of different parameters on coating properties are evaluated and necessary conditions for resistant coatings independent from coating setup are identified. The findings could lead to a more extensive understanding beneficial to similar challenges concerning process transfer between different PECVD setups. Additionally, a concept for process monitoring could be derived, which is of great interest regarding a commercial application of such resistance coatings.

Marcel Rudolph, project T4 of the SFB-TR 87

Plasma-driven biocatalysis – challenges and how to overcome them

Non-thermal plasmas have emerged as an interesting source for reactive nitrogen and oxygen species (RONS) to drive biocatalytic reactions. Previously, we were able to show that enzymes like the unspecific peroxygenase (UPO) can use hydrogen peroxide (H_2O_2) generated by a DBD device to convert organic compounds with high selectivity [1]. In this initial study, however, several challenges occurred that needed to be addressed. The major challenge was that the employed enzymes were quickly inactivated by the plasma treatment, presumably by short-living RONS. Immobilization of the enzyme proved to significantly increase the lifetime of the enzyme under plasma treatment, but also resulted in lower conversion rates of the substrates. We therefore investigated whether protective proteins could be used in conjunction with unbound enzymes in plasma-driven biocatalysis. One of the most deleterious RONS produced by plasmas in ambient air is superoxide (O_2^-), which attacks structures in enzymes necessary for their activity. Since O_2^- also occurs naturally in organisms living aerobically (in oxygen-containing environments), natural protection strategies against O_2^- exist. Among these protection strategies are superoxide dismutases, which are enzymes that directly convert O_2^- to H_2O_2 and molecular oxygen. Being able to harness superoxide dismutases for plasma-driven biocatalysis would present two advantages: 1) harmful O_2^- is scavenged and 2) more of the required H_2O_2 is supplied for the reaction. However, when superoxide dismutase A (SodA) from *Escherichia coli* (*E. coli*) was tested for use in plasma-driven biocatalysis, we found that SodA was also quickly inactivated by the plasma and did not benefit the reaction progress (Fig. 1a) [1,2]. Activity and mass spectrometry measurements after plasma treatment indicated that RONS caused modifications of amino acid side chains in SodA, which in turn distorted the active site of the enzyme and reduced its activity (Fig. 1b). In addition, degradation of the protein occurred, adding to the inactivation of SodA.

As scavenging of O_2^- did not significantly improve the biocatalytic reactions with plasma, we turned to other methods of enzyme protection. Chaperones are proteins that stop other proteins from aggregating after unfolding and have been shown to be beneficial for the survival of bacteria under plasma treatment [3]. When these proteins were used in plasma-driven biocatalysis, they, again, did not improve the lifetime of the catalytic enzymes under plasma treatment [4]. Similarly, two other approaches, namely the use of chemical scavengers to specifically detoxify damaging RONS like ·OH or ·OOH and the use of different gas atmospheres for plasma ignition, did not protect UPO either. Therefore, immobilization presented the most promising approach and was investigated in-depth to increase the lifetime of proteins exposed to plasma. Interestingly, we found that the mode of immobilization and type of support material greatly influence the effect of the plasma on UPO. Testing different support surfaces, in a new set of experiments, the lifetime of UPO was further increased compared to the initial immobilization experiment (Fig. 2).

With the improved immobilized UPO, we set out to scale-up the reaction by using a microscale atmospheric pressure

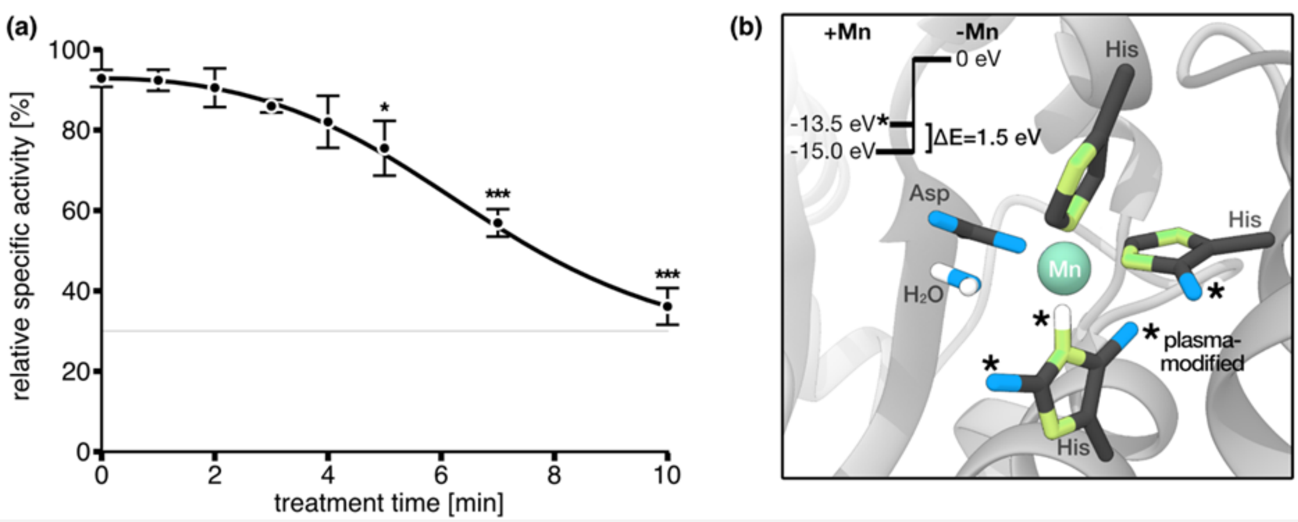


Fig. 1 Impact of DBD plasma on bacterial superoxide dismutase A (SodA) [2]. (a) SodA was treated with DBD plasma and afterwards the residual enzyme activity was determined. (b) Active center of SodA. Mass spectrometric analyses in combination with Coupled Cluster Calculations revealed that plasma-induced oxygenations of two histidine amino acids (marked with asterisks) in the protein's active center are causing a reduction in the binding affinity of the protein to an essential manganese ion (ΔE = 1.5 eV). This ultimately causes protein inactivation.

plasma jet (µAPPJ). Using the µAPPJ, we increased the reaction volume from µl to ml scale while retaining a high conversion rate of the substrate [5]. In addition, after a reaction time of 80 min, the enzyme suffered virtually no inactivation, indicating that this setup can be run for extended periods of time. The product of this reaction scheme proved to be highly pure and was not modified by plasma treatment. In summary, while plasma-driven biocatalysis depends on immobilized enzymes, the efficiency of the system was improved significantly and is likely to be improved further.

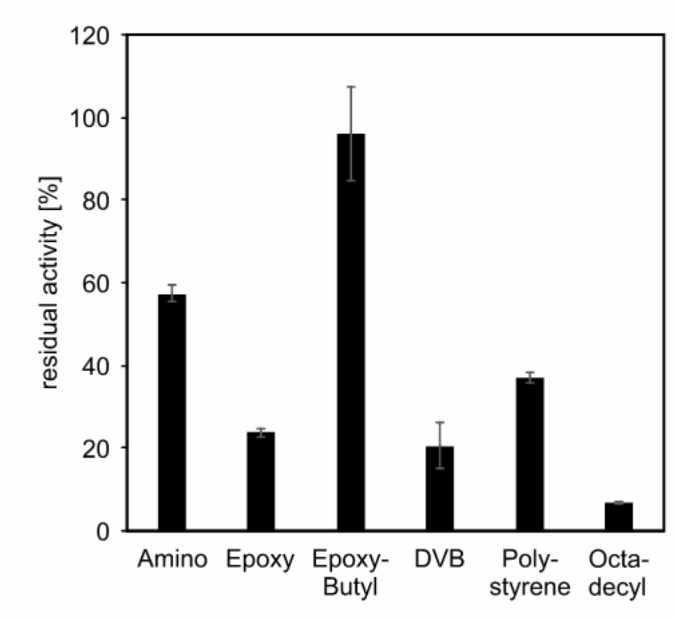


Fig. 2 Activity of UPO immobilized on different supports after plasma treatment [4]. UPO was immobilized to the respective supports according to the manufacturers' instructions. Samples of immobilized UPO were treated with the Cinogy PlasmaDerm device and the activity was measured in a standard colorimetric assay. Residual activity is displayed as the ratio between activity before and after plasma exposure.

[1] Abdulkadir Yayci, Álvaro Gómez Baraibar, Marco Krewing, Elena Fernandez Fueyo, Frank Hollmann, Miguel Alcalde, Robert Kourist, Julia E. Bandow, *ChemSusChem* **2020**, *13*, 2072.

[2] Marco Krewing, Christoph K. Jung, Elena Dobbelstein, Britta Schubert, Timo Jacob, Julia E. Bandow, *Plasma Processes and Polymers* **2020**, 2020;e2000019.

[3] M. Krewing, J. J. Stepanek, C. Cremers, J.-W. Lackmann, B. Schubert, A. Müller, P. Awakowicz, L. I. O. Leichert, U. Jakob, J. E. Bandow, *Journal of the Royal Society, Interface* **2019**, *16*, 20180966.

[4] Abdulkadir Yayci, Tim Dirks, Frank Hollmann, Friederike Kogelheide, Peter Awakowicz, Julia E. Bandow, *Journal of Physics D: Applied Physics* **2021**, 54:035204.

[5] Abdulkadir Yayci, Tim Dirks, Frank Hollmann, Friederike Kogelheide, Peter Awakowicz, Julia E. Bandow, *ChemCatChem*, **2020**, 12 (early view: DOI: 10.1002/cctc.202001225).

Abdulkadir Yayci, project B8 of the CRC 1316

Workshop

Gender equality seminar online

PHD... AND NEXT?

A question that probably a lot of scientists ask themselves at some point during their PhD studies. To find an answer to this question or at least to get a better impression of our career options, we attended an online workshop which dealt exactly with this question. 'We' were eight PhD students from Bochum, Ulm and Aachen who participated in the workshop, which was given by Karin Bodewits from NaturalScience.Careers and financed by the SFB gender equality means. The online workshop stretched across one week in September and included one individual coaching session for each PhD student. During this course, we were introduced to different job options that included not only the widely known careers of academia and R&D in industry, but also less obvious career choices, like journalist, science illustrator, communicator, patent lawyer, advisor for the government or management consultant. On the one hand, we went over the skills that are required for the different job positions and on the other hand, we discussed the skills that many students develop during their PhD. Furthermore, we learned about the important criteria of a convincing CV and in the individual session, we received valuable feedback on how to improve our personal CV. It was a very interesting workshop and I am sure that many of the insights we gained during this week will become useful when we make decisions about our future career path.

Lena Patterer, project A3 of the SFB-TR 87

New group leader plasma interface physics Jun.-Prof. Golda

The establishment of new research groups is always good news. They support the ongoing scientific activities in the existing groups and bring new impulses in other scientific directions.

Today, we would like to present Jun.-Prof. Judith Golda, who will also join the CRC 1316 with new projects and support the success of the scientific work within this research centre. Her research group focuses on the interface of plasma and surface.

Dear Jun.-Prof. Golda, welcome back to the Ruhr-University Bochum. You are now leading a junior research group after your PostDoc time at Kiel University. What are your first (scientific) goals in Bochum?

Initially, I want to establish a research team. I am looking for people who are willing to push the edges of science, working hand in hand with their colleagues. As a group leader, you are only as good as your group.

Scientifically, I want to have a closer look at the processes within the plasma interface. This is the region where direct interaction between plasma and materials, e.g. solid and liquid surfaces or biologic substrates, takes place. Which mechanisms are important and how can we develop diagnostic techniques dedicated to fundamental insight into this region?

What was the main motivation to take over a research group within a such interdisciplinary research field?

I am a curious person – I am always looking for new challenges and things to learn. This interdisciplinary research field gives me the opportunity to broaden my knowledge. Additionally, I enjoy working with other people. This opens up completely new perspectives and often brings momentum to a project. The combination of different expertise can sometimes even initiate completely new scientific fields.

What is your research question of your contribution to the work of the CRC 1316?

In the CRC, I will work on different projects. All of them are related to plasma interface physics: In one of the new subprojects, we are trying to find out how we can rationally design a plasma setup which serves best our needs in terms of tailored radical production for biocatalysis. To do this, we have to understand the complete reaction path ranging from the feed gas via the plasma, the effluent into the liquid and the substrate.

Additionally, we are going to investigate the plasma-surface interaction of microcavity plasma arrays and an RF atmospheric pressure plasma jet with different materials such as catalysts.

What expertise will you contribute to the CRC 1316?

The CRC 1316 consortium already consists of excellent researchers. With my expertise, I will contribute to bridge the gap between plasma physics and biocatalysis and share my knowledge about plasma diagnostic techniques.

What do you think is the main challenge for the work within the CRC 1316?

In my opinion, one of the main challenges is the interdisciplinary topic of plasma catalysis. The expertise of engineers, physicists, chemists and biologists is required here, to drive research forward. Especially the communication between the disciplines, e.g. the language as well as the different work environments in the laboratories has to be overcome.

Last week, I had the chance to attend the CRC 1316 fall meeting and was impressed by how far the consortium has come so far.

What do you do besides your passion for physics?

I like doing sports. This includes running and climbing, but also team sports. After a knee injury, I had to take it easy and switched to canoe polo in Kiel - here in Bochum, I will see what possibilities are available and what looks like fun.

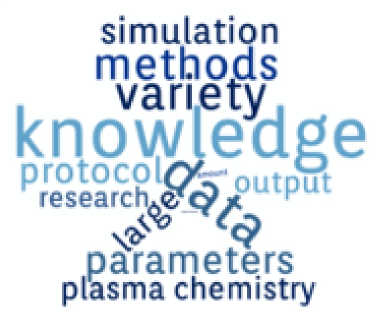
Thank you.

interview by Marina Prenzel, public relations

Research data management established as subproject for next funding phase

The scientific practice of storing research data has existed for years. The current work in the field supports the lived practice to a new level, which is currently being established in the scientific community.

In order to support the new developments, it is therefore necessary to become active in various areas. CRC 1316 and SFB-TR 87 are therefore supported by the following activities on research data management:



Repository

As a main aspect within the CRC 1316, research data are published within a platform (rdpcidat.rub.de), which is accessible via the web. Here, journal papers and their original data can be published and stored. To intensify the quality of these data, the central administration of RUB will support the to transfer of the repository to the central storage on campus RUB during the second funding phase of the consortium.

RDMS-FDM RUB CRC 1280

A collaboration based on regular exchange with the CRC 1280 has been started to share experiences or concepts.

NFDI4Phys

The CRC 1316 will be listed as a use case in the NFDI4Phys consortium. The application is planned for September 2021. A contribution in the context of data literacy has been registered.

QPTDat cooperation

Participation in regular workshops works well. We were able to contribute to the development of metadata schemas with the help of the scientists in the CRC 1316. Here, in the area of diagnostics, the metadata schemas will be added next to the repository, which will then also be visible in the Bochum repository.

RDM trainings

Concrete steps to further introduce the scientists to the topic of research data management will be a RDM training, which will be conducted by the corresponding department of the RUB. The date will be around the second quarter of 2021.

In case, you need further information regarding this topic, please contact *rd-plasma@rub.de*.

Marina Prenzel, SFB-TR 87 and CRC 1316

Upcoming Events of the CRC 1316 & SFB-TR 87

18-19 FEB
SFB– TR 87
Virtual Project Meeting

18-19 MAR
Workshop:
How do different gender codes influence our communication? What can we learn from the other sex?

21-24 MAR
Conference:
1st Frontiers in Plasmas in Industry and PT20

21-22 APR
CRC 1316 and SFB-TR 87 —
MGK Colloquium

7-9 JUN
SFB-TR 87
Project meetings A, B, C

10-12 NOV
SFB– TR 87
Project meetings A, B, C

Please check the CRC 1316 and SFB-TR 87 websites for up-to-date information on the events.

Controlled reactive HIPIMS: Effective technique for low-temperature deposition of tunable deposition of tunable oxynitrides and functional oxides

Prof. Jaroslav Vlček from the University of West Bohemia presented a seminar on “Controlled reactive HiPIMS: Effective technique for low-temperature deposition of tunable oxynitrides and functional oxides" on 17 September 2020. The presentation was focused on the combination of HiPIMS with a pulsed oxygen flow controller in order to maximize the degree of dissociation of reactive N_2 and O_2 gas molecules in the plasma. This unique capability enables e.g. the tuning of Al-O-N thin film chemical compositions: while molecular N_2 and O_2 exhibit significantly different reactivities, $Al_{0.45}(O_{0.49}N_{0.51})_{0.55}$ was grown at equal flows of N_2 and O_2. In the framework of thermochromic materials, Prof. Vlček demonstrated that the employment of this pulsed oxygen flow control enables the scalable low-temperature synthesis of $(V_{0.982}W_{0.018})O_2$ at 330°C without any substrate bias potential. Such thin films exhibit a transition from a monoclinic, semiconductive to a tetragonal, metallic phase at a temperature of 20-21°C and are therefore extremely promising for application on smart windows. Finally, the high-rate deposition of optically transparent HfO_2 thin films with up to 200 nm/min were realized at a substrate temperature of < 165°C and floating substrate bias potential. These findings were very interesting for the plasma-surface model of SFB-TR 87.

Marcus Hans, project A3 of the SFB-TR 87

In-situ XRD during magnetron sputter deposition and arc deposition, and in-operando XRD during high-speed cutting

Prof. Jens Birch from Linköping University gave a seminar on 28 October 2020. In the first part, he introduced the audience to the concept of high-energy X-ray scattering and presented the advantages of this research method. High-energy synchrotron X-rays do not only allow structural investigations within a deep penetration depth of the sample material but also require only a short acquisition time. Therefore, investigations of dynamic processes are possible, like time-resolved *in-situ* sputtering experiments and also so-called *in-operando* measurements. For this purpose, Prof. Birch’s group set up a UHV deposition system at DESY in Hamburg which allows *in-situ* investigations of film growth under real industrial conditions. Additionally, the setup of a custom-made lathe was presented which allows the structural study of tool-chip and tool-workpiece contact zones during cutting. *In-operando* stress analysis of TiNbAlN arc-coated WC-Co cutting tools revealed that at higher cutting speed (320 m/min) a less compressive residual stress state was identified on the tool edge compared to the operation at lower cutting speed (235 m/min). This is explained by the larger relaxation of intrinsic stresses during the high-speed cutting scenario. All in all, the workshop gave an interesting overview of the possibilities of high-energy XRD investigations of hard coatings and was therefore especially of relevance for the mechanical model of SFB-TR 87.

Lena Patterer, project A3 of the SFB-TR 87

Autonomous crack healing in MAX phase ceramics

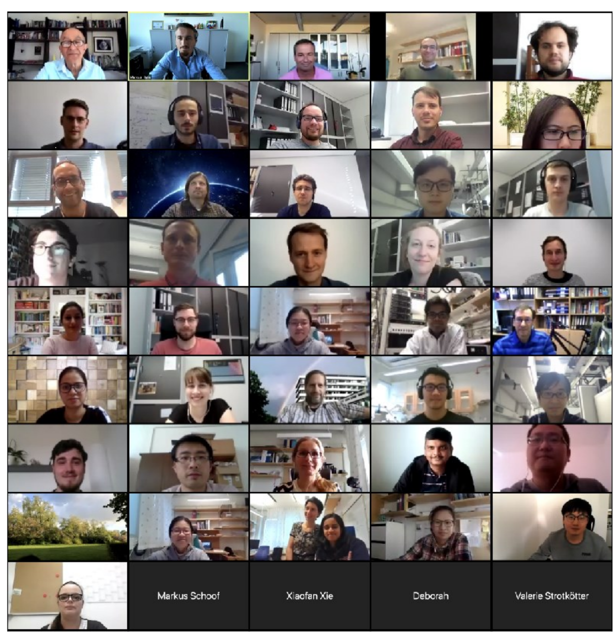
Prof. Willem G. Sloof from the Delft University of Technology, Netherlands presented the seminar "Autonomous crack healing in MAX phase ceramics" on 29 October 2020. The talk started with the concept of extrinsic self-healing which is achieved by embedding sacrificial particles in the material matrix. These sacrificial particles are supposed to react with oxygen from the ambient at elevated temperatures and the formed oxides can fill the open cracks and terminate the crack propagation. As an example he demonstrated that TiC particles in ceramic matrix materials are able to fill cracks by formation of TiO_2. Prof. Sloof also introduced a kinetic model, which aimed to estimate the healing process time of the alumina matrix with open cracks and embedded Ti particles above 700°C. The experimental data showed good agreement with the model. In the second part, Prof. Sloof focused on the intrinsic self-healing of MAX phases, where the embedded particles are not needed any more. Oxygen selectively reacts with the A element (usually Al or Si) in the MAX phases, forming oxides. Moreover, the group of Prof. Sloof studied and quantified the self-healing behavior of Ti_2AlC by a 4D *in-situ* synchrotron X-ray tomographic microscopy. The temporal and spatial evolution of cyclic cracking and healing were instantaneously captured. These insights were in particular relevant for the SFB-TR 87 transfer project T1.

Yu-Ping Chien, project T1 of the SFB-TR 87

Fundamentals of sputter deposition

Prof. Ivan Petrov from the University of Illinois gave a workshop on 17 and 18 September 2020. In this workshop Prof. Petrov covered the key concepts of sputter deposition from the basics of kinetic theory of gases to the capability of tuning the micro-, nano- and even further the atomic structure of thin films by independently controlling the fundamental parameters in ion-assisted physical vapor deposition: ion flux and kinetic ion energy. Firstly, within a wide range of transition metal nitrides such as TiN, TaN, and HfN, the advantage of high fluxes of low energy ions in formation of dense epitaxial structures was discussed. On the other hand, it has been demonstrated that not only the energetic ion irradiation could be employed to form non-columnar equiaxed structures for high temperature oxidation resistance applications, but also segregation of a second incommensurate phase such as YN or CeN in TiN would lead to formation of equiaxed films with low residual stress and defect densities. In the next section, the Hybrid process (combination of DCMS and HPPMS) was introduced which has the capability of separating the film forming species in time and energy domains. Therefore, growth of an unprecedented Al supersaturated single phase cubic $V_{0.25}Al_{0.75}N$ was enabled by implementing this approach due to activation of bulk diffusion and incorporation of only desired energetic Al ions from the plasma into the growing surface. Finally, modeling of TiN(001) film growth by ab initio and classical Molecular Dynamics was demonstrated to simulate the real deposition conditions. It was interestingly observed that the low energy (10 eV) high flux of ions leads to the restructuring of the atoms on the surface and consequently epitaxial growth of TiN as it was observed experimentally. This workshop was highly in line with SFB-TR 87 plasma-surface and mechanical models.

Soheil Karimi, project A3 of the SFB-TR 87



IMPRESSUM

Public relations SFB-TR 87 & CRC 1316

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