NEWSLETTER

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SFB-TR 87

SFB 1316 Transient Atmospheric Plasmas
from plasmas to liquids to solids

FOREWORD

You are holding the current newsletter of the Collaborative Research Centers SFB-TR 87 and CRC 1316 in your hands. Also this time we want to communicate an attractive mix about developments in the two Collaborative Research Centers.

Two further transfer projects in the SFB-TR 87 have started and promise a great collaboration with corresponding industrial partners.

In the last months, many on-site events could take place again, but also online or hybrid events were made. Here, the large number of activities on the part of the MCh group at the RWTH is particularly noteworthy.

Moreover, we were able to profit here in the area of public relations, since further actions such as Girl's Day or the school girls' project week could again be held on the premises of the RUB.

A highlight of the event series was the summit meeting of the SFB-TR 87 at the Eibsee. The findings of the last twelve years on the topic of high performance plasmas were underlined by lectures in a two and a half day meeting.

We hope you enjoy reading this newsletter.

Marina Prenzel, public relations of the SFB-TR 87 & CRC 1316

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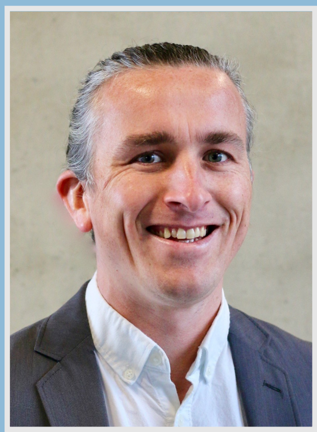
* Title page image: Particle Beam Experiment for Secondary Eletron Emission Coefficent Determination

Prices, Awards and Honors

SFB-TR 87 scientist elected as member of the Early Career Advisory Board of the journal Surface and Coatings Technology

Dr.-Ing. Marcus Hans has been elected as member of the Early Career Advisory Board (ECAB) of the journal Surface and Coatings Technology.



This advisory board has been initiated to promote outstanding early career researchers and engage them in a path towards editorial services and contributions. The ECAB program starts on 1 January 2022 and a typical term for ECAB members is 2 years with a possible renewal for a second term.

Main responsibilities of the ECAB members include (i) Conducting reviews for a certain number of papers annually, (ii) Submitting at least two manuscripts within the term (which are subject to external peer review as with any other submission), (iii) Acting as an ambassador to promote the journal via social media, conferences, and other channels, (iv) Providing consultation to the editors at their request, and (v) Assisting with special issues under the guidance and discretion of the editors.

Philipp Grosse's publication on electrochemical CO_2 reduction in Nature Communications

A team of researchers from the Department of Interfacial Sciences at FHI Berlin has discovered how changes in the structure of copper catalyst particles during electrochemical CO_2 reduction affect their catalytic performance. This should lead to the development of new catalysts that convert the greenhouse gas CO_2 into useful chemicals. Researchers around CRC member Philipp Grosse from project B1 published their work in the journal Nature communications.

The could show how the initial number of catalysts particles, their size and density on the support electrode surface is not a reliable indicator of the actual number of particles present during reaction. More importantly, Philipp Gosse and colleagues show that by optimizing the design of the pre-catalyst structures, the structural evolution under working conditions is influenced and thus also their selectivity. This is also important for the electron microscopists. This is a significant advance in the field of liquid phase electron microscopy.

Marina Prenzel, public relations of the SFB-TR 87 & CRC 1316

ION-INDUCED SECONDARY ELECTRON EMISSION OF OXIDIZED NICKEL AND COPPER STUDIED IN BEAM EXPERIMENTS

Rahel Buschhaus, Marina Prenzel and Achim von Keudell

In project C7 of the SFB-TR 87 low pressure plasma-surface interactions are investigated. A particle beam experiment is applied to disentangle the process of ion-induced secondary electron emission from all other processes (such as sputtering or electron- and photon-induced electron emission).

When a plasma is in contact with any kind of surface (for instance electrodes or targets for treatment), several plasma-surface interactions occur. An important interaction is the process of electron emission upon ion impact. The amount of released surface electrons per impinging ion is called ion-induced secondary electron emission coefficient γ (SEEC). This coefficient is strongly influenced by the chemical condition of the surface. For instance, it is known [1] that γ tends to be higher for surfaces upon gas adsorption. γ for gas adsorbed surfaces (e.g. oxidized) is of special interest e.g. when modeling a reactive plasma: γ is a key input parameter for PIC simulations. However, a study of γ for well-defined surface conditions is mostly missing in the literature.

In our recent study, we determined γ for both, nickel, and copper in a beam experiment of three different surface conditions: (1) clean, (2) untreated/air-exposed, and (3) in-situ intentionally oxidized surfaces.

The surface conditions were analyzed ex-situ in collaboration with Marina Prenzel (XPS in project C7) and Felix David Klute (SEM in project B2) as well as preliminary measurements by Sabrina Schwiderek (XPS in project B3) giving the following surfaces to be analyzed:

A) Clean Ni and Cu: are indeed clean after sputtering with Argon ions.

B) Untreated/air-exposed Ni and Cu: natural oxide + contaminations of H, C, and N.

C) Intentionally oxidized Ni and Cu: pure oxides with stoichiometries of NiO and Cu_2O and oxide thickness of 4-5 nm.

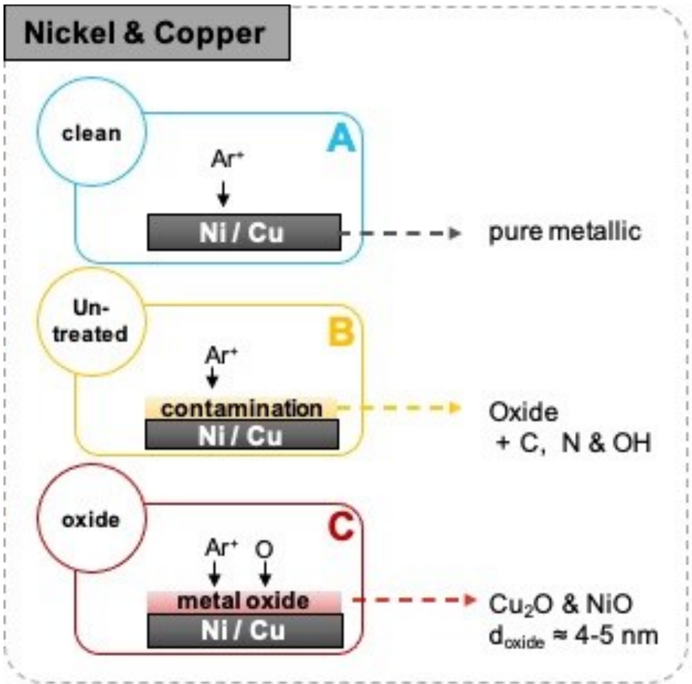


Figure 1: Scheme of the prepared surfaces.

The main results (see figure 2) are:

1. We can precisely determine γ for different surface conditions in a broad energy range (300 eV...10 keV).

2. For clean and untreated nickel and copper, we have a good agreement with the literature. Thus, our measuring approach is working well.

3. The least electrons are released from a clean surface, the most electrons from an untreated surface.

4. γ of air-exposed and intentionally oxidized metals are not identical. This behavior can be explained by analyzing the ongoing processes upon ion impact in the material. In a nutshell: for any kind of oxides (air-exposed or purely intentionally oxide) the electron generation inside the material is more efficient compared to a clean surface. Therefore, γ of air-exposed and intentionally oxidized metals is higher compared to a clean surface. However, on the other hand, upon

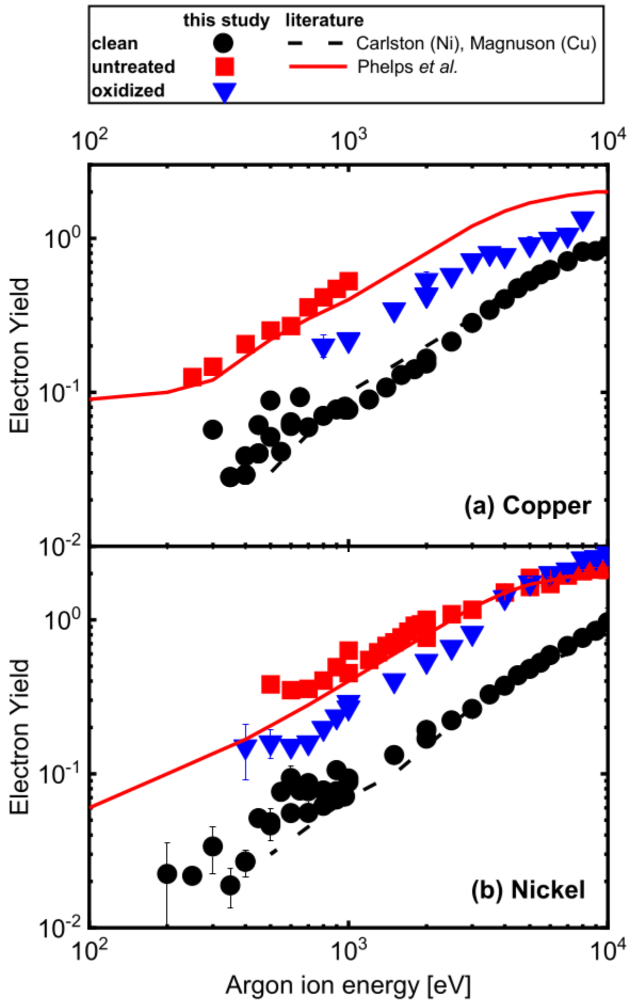


Figure 2: Electron yields for (a) Copper and (b) Nickel depending on the argon ion energy.

gas adsorption, the work function of a material increases, and thus the electron release is inhibited. As H, C, and N are less electronegative with respect to O, the work function of air-exposed surfaces is further reduced compared to pure oxide. Thus, the electron release of air-exposed surfaces is higher and therefore the relationship γ (air-exposed) > γ (intentionally oxidized) is occurring.

Take-home message:

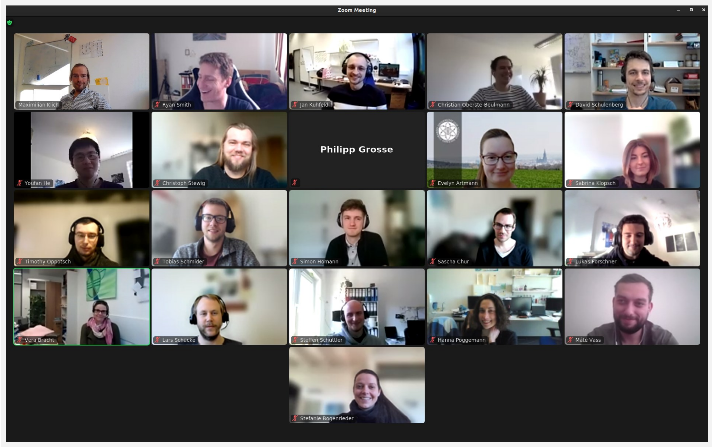
When you are modeling your plasma and searching for appropriate electron coefficients, please pay attention as γ strongly depends on the surface conditions.

[1] A. V. Phelps and Z. L. Petrovic, Plasma Sources Sci. Technol, vol. 8, 1999

This work has been published as R. Buschhaus et al Plasma Sources Sci. Technol. 31, 025017 (2022).

Rahel Buschhaus, project C7 of the SFB-TR 87

MGK Colloquium



With the start of the second funding period, all PhD students of the projects within the CRC 1316 were invited to participate in the annually MGK colloquium. The colloquium was held online at 7th and 8th of March 2022 and was organized by Maximilian Klich (project A8) and David Schulenberg (project A4).

The colloquium served as an introduction of the many new PhDs joining the CRC 1316 in its second funding period. Without the participation of project leaders it achieved a casual atmosphere for sharing scientific knowledge and interests between the PhD students. Here, they could introduce themselves and their projects as well as give a short summary about their projects achievements and future plans through talks or a poster presentation. Leading the talks regarding the different research topics modelling, DBD/RF discharges and plasma in liquids were the invited speakers which generated a well rounded experience.

The new funding period also required a few elections, namely the position of the PhD speaker formerly held by Maximilian Klich, as well as a position in the CRC 1316 gender board held by Lars Schücke (project A7) and Katharina Grosse (project B7). The newly elected PhD speaker is David Schulenberg and Stefanie Bogenrieder (project B4) as well as Lukas Forschner (project B12) are the new gender board representative.

Sascha Chur, project B2 of the CRC 1316

Plasma for School Students

Girls' Day 2022

On April 28th, the annual Girls' Day took place. Offering a 5-hour hands-on workshop on plasma physics, female students could dive into university physics as well as learn more about science, studying and career options pursuing studies in physics. During the workshop, the school students first got to know the basics of plasma – what does it consist of, how can we influence its behaviour and which characteristics does it have. Following this rather theoretical part, the school students worked on the sputter coater, making samples to analyse with a profilometer and identify the thickness of the surface coating from the sputtering process. The aim of the Girls' Day is to offer female school students an insight into technical and scientific careers and motivate more school students to choose a degree in a MINT-subject. We also aim at reducing prejudices and fears towards a physics degree.

Maike Kai, public relations for the SFB-TR 87 & CRC 1316

Project Week during Easter Break

During the first week of the Easter break, the project weeks for female high school students (in German Schülerinnenprojektwoche) took place and opened the doors towards plasma physics, astronomy and physics in medicine for school students grade 8 to 10.

Hosting three projects, the offer is continuously expanding after the Corona lockdown. During the project week, students attended a lecture given by PD Dr. Horst Fichtner on '*news from the edge of the solar system*', visited the Planetarium in Bochum and worked on scientific projects during their workshops. The outcomes of the research projects were presented in a poster session followed by a quiz and shared lunch, which formed the conclusion of the week.

To lower the entry barrier of the project week and offer school students the chance to participate no matter of their financial status, some changes were implemented as a trial. School students who do not own a ticket for public transport had the option to receive a ticket for transportation to and from university. Also, meals were newly included in the project week. While only breakfast used to be supplied, students could now share a free lunch in the campus dining hall, enhancing the group dynamics and their feeling of belonging in the group.

The feedback to this changes were positive according to the feedback of the participants, so that the changes will be continuously adapted to the program of the project week The project week in autumn will presumably take place with four projects at full capacity.

Maike Kai, public relations for the SFB-TR 87 & CRC 1316

Research Seminar Report

Within the last months, several research seminars took place at the Chair of Materials Chemistry, RWTH Aachen.

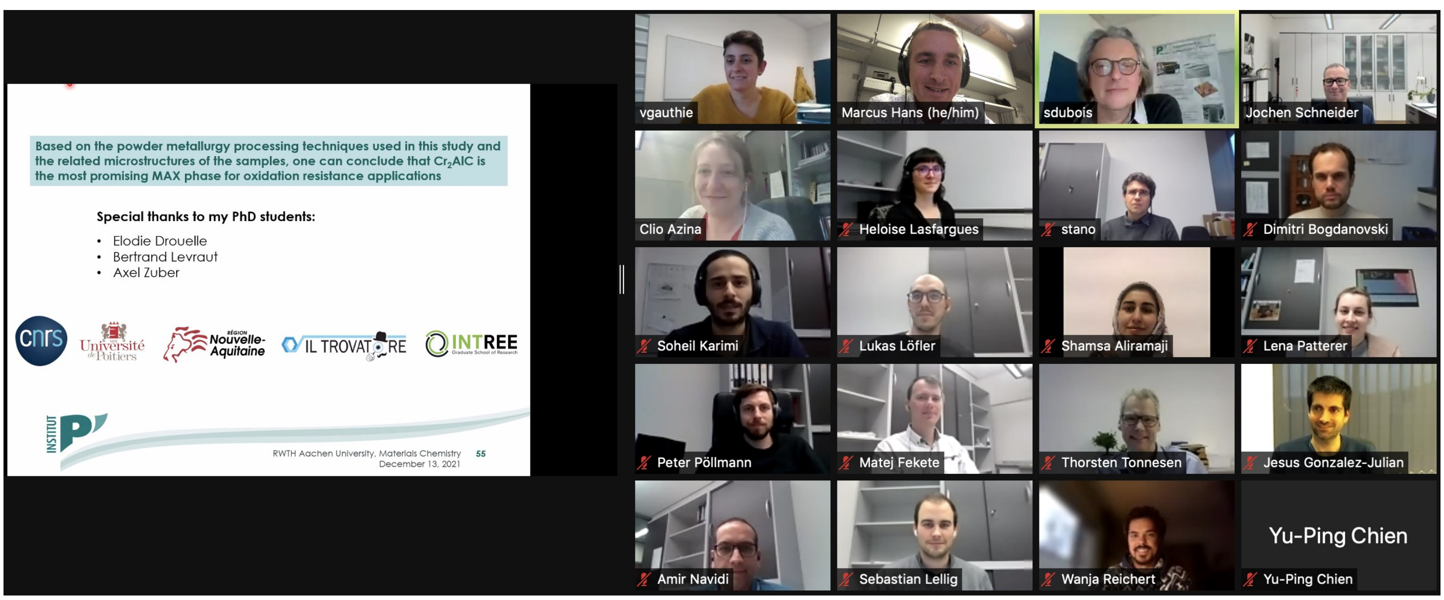
Recent Advances in MAX Phase Solid Solutions & High Temperature Oxidation of Alumina-Forming MAX Phases

Prof. Sylvain Dubois and Prof. Veronique Gauthier-Brunet from Université de Poitiers gave a two-part workshop on 13 December 2021 via Zoom. Prof. Dubois is currently the director of the Department of Physics and Mechanics of Materials (Institute PPRIME) and Prof. Gauthier-Brunet is associate professor at this institute.

Prof. Dubois started with a comprehensive overview of existing MAX phases and their properties before introduction of a new quaternary MAX phase solid solution. From a thermodynamic point of view, a possible stabilization of the solid solution can be achieved due to the configurational entropy. The MAX phases family has been expanded by using Cu to substitute the Al in the Ti_3AlC by the powder metallurgy processing. According to the X-ray diffraction data, lattice distortion was caused due to the replacement of Al by Cu which resulted in the symmetry reduction and formation of a monoclinic structure.

In the second part, the relation between the powder metallurgy route which affects the microstructure of the materials and the oxidation behaviour of the MAX phase was discussed by Prof. Gauthier-Brunet. $Ti_{n+1}AlC_n$ (n = 1 or 2) and Cr_2AlC were studied. Coarse-grained material was synthesized by hot isostatic pressing (HIP), while fine-grained MAX phases were produced by spark plasma sintering (SPS). After oxidation at 1000°C, Ti_2AlC showed better oxidation resistance than Ti_3AlC_2 because of higher Al concentration. Due to the large number of grain boundaries which provide diffusion paths for Al^{3+}, the protective Al_2O_3 layer can be formed in the fine-grained Ti_2AlC sample, while the coarse-grained one has a mixture of non-protective TiO_2 and Al_2O_3 layer. However, for the Cr_2AlC samples, the coarse-grained, fine-grained, and single crystal bulk Cr_2AlC showed no significant differences with respect to oxide scale formation. A continuous Al_2O_3 layer was found after oxidation in the temperature range between 800 and 1400°C. Finally, Prof. Gauthier-Brunet also showed that the grain orientation and surface roughness both influence the thickness of the Al_2O_3 layer. These findings are relevant for the interaction model of SFB-TR 87.

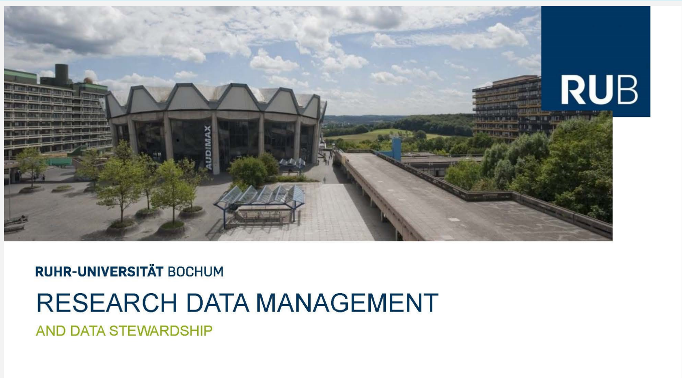
Yu-Ping Chien, project T1 of the SFB-TR 87



Exchange Research Data Management UA Ruhr & Oulu

Under the slogan "Mining of research data instead of coal" the UA Ruhr organized an international knowledge exchange on data management with researchers working as data stewards at the University of Oulu, Finland on 11th and 12th May. The event was hosted in the convention center of Ruhr University Bochum and by zoom.

The local structures supporting research data management at the UA Ruhr universities were presented and experiences on advice, training and data management plans, and discuss best practices were shared.



Furthermore, an exchange between the CRCs CRC 1280 and CRC 1316 as well as the partners from UA-Ruhr and the Finnish guests took place. Here researchers and data stewards as well as data experts from the consortia were brought together.

The event was a great success, as the structures on both sides differ, but the challenges of the individual actors in the field of data management are identical. Thus, many interesting experiences could be exchanged. Due to the success, a return visit to Oulu is now being planned to continue the exchange.

Marina Prenzel, INF of the CRC 1316

Contributions of PE plastic packaging

Lara Kleines, Philipp Alizadeh, Rainer Dahlmann

The SFB-TR 87 transfer projects bring findings from fundamental research into industrial applications. The projects T06 and T07 are aiming to enhance the application of circular resource management by the means of plasma technology.

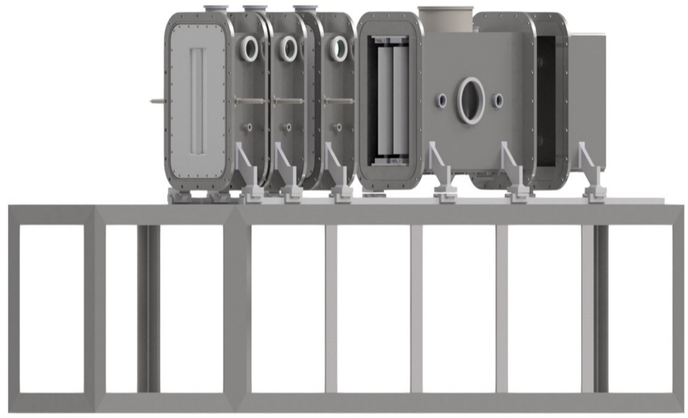


Figure 1: Plant development design

Flexible packaging must harmonise a high level of product protection with complex supply chains. Packaging solutions made of multi-material composites are therefore particularly widespread. The individual layers consist of different plastics, metallised layers or paper. After use, these individual layers are difficult to separate and thus often unusable for material recycling. The application of plasma-polymer coatings is one way of functionalising plastic films in a variety of ways without impairing their recyclability. However, due to comparatively high process costs, the technology has not yet been established in the packaging film market.

The aim of the transfer project T06 “In-Plasma-Air2Air” from SFB TR 87, which started in October 2020, is therefore to develop an experimental reactor that significantly reduces the downtime due to cleaning and evacuation of the process chamber. This is to be achieved, on the one hand, by continuously feeding and discharging the film by means of sealing modules and, on the other hand, by enveloping the plasma zone by the substrate.

CVD TECHNOLOGY TO THE CIRCULAR ECONOMY OF

In order to achieve this ambitious project goal, a joint project is currently underway with AEPT (RUB), Bühler Alzenau GmbH, Constantia Pirk GmbH & Co. KG, Pfeiffer Vacuum Components & Solutions GmbH, Reifenhäuser Cast Sheet Coating GmbH & Co. KG and SIG Combibloc Systems GmbH, the expertise from decisive disciplines of packaging, vacuum and plasma technology as well as plant engineering for coating reactors has been brought together.

The research project pursues a modular plant design and is being developed with scalability in mind to favour rapid implementation in industry (Figure 1).

The European Commission's Plastics Strategy, published in January 2018, sets the goal to recycle at least half of the plastic waste by 2030 and thus to substantially increase the share of recyclates used in newly produced plastic products. Although the packaging sectors demand in Europe has the highest share (almost 40%) compared to other sectors, the success of the European initiative to increase the use of recyclates is currently hindered by, among other things, the very limited possibility of using recycled plastics in the food sector. One of the main reasons for this is the risk of migration of chemical substances from the used packaging into the food and a subsequent lack of safety of the food contact materials evaluated in an assessment of safety by the European Food Safety Authority (EFSA). Sufficient product protection in terms of toxicity, taste and odour changes as well as contamination of various kinds cannot be guaranteed for most materials especially when using post-consumer recyclates (PCR) other than polyethylene terephthalate (PET).

The aim of the transfer project T07 “RezyPlas” is to explore and further develop the potential of highly functional PECVD coating systems as migration barriers for contaminants from recyclates. Thereby the focus lies on non-PET materials such as polypropylene (PP), as this is where the biggest hurdles lie for the use of recyclates in food contact. Basic research as well as application-oriented experiments and theoretical models are being used to understand different effects and processes in the system consisting of recycled plastic, the PECVD coating and a foodstuff. The use of functional migration

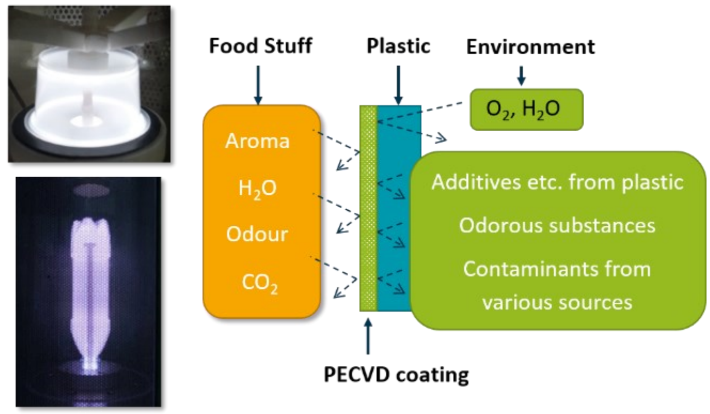


Figure 2: Using PECVD coatings as migration barriers for contaminated recyclates in food contact.

barriers in this case not only has a high level of potential from a process technological perspective, but also from a regulatory point of view, as EU regulations declare that behind a functional barrier, non-authorised substances may be used, provided they fulfil certain criteria and their migration remains below a given detection limit.

Methodologically, in a first step, test substances are used to simulate the contamination of the recyclates and their uptake by food. Suitable coating systems are then developed on these contaminated materials, which requires intensive analysis due to the unknown surface properties of the recyclates. These coating systems are tested in extensive migration analytical studies for their suitability for migration reduction. In addition extensive interface analysis is carried out to generate insights into the migration processes in the interface between recyclate and coating.

In this project the research work is supported by the industry partners Gizeh Verpackungen GmbH & Co. KG and Der Grüne Punkt - Duales System Deutschland GmbH. The University of Paderborn is also providing support with its analytical expertise in terms of interface analytics.

Nanolamellar Chemical Vapor Deposited fcc-$Ti_{1-x}Al_xN$

Dr. Michael Tkadletz, head of the Advanced Microstructure and Nanostructure Characterization group at Montanuniversität Leoben gave a Zoom workshop on the topic of 'Nanolamellar chemical vapor deposited fcc- $Ti_{1-x}Al_xN$ – History, peculiarities and future perspectives' on 1 December 2021.

The presentation focused on fcc-$Ti_{1-x}Al_xN$ coatings with high Al contents which are often used for cutting tools. A high global Al-content in fcc-$Ti_{1-x}Al_xN$ coatings is beneficial for the oxidation resistance and hardness, ensuring a superior cutting performance compared to conventional protective $Ti_{1-x}Al_xN$ coatings. These conventional coatings deposited by physical vapor deposition (PVD) are usually limited to an Al content x of ~ 0.6-0.7 on the metal sublattice and for higher Al concentrations a fcc/wurtzitic dual-phase starts to form, reducing the mechanical properties of these coatings. In contrast, an Al metal ratio x of ~ 0.8 has been reported for chemical vapor deposited (CVD) $Ti_{1-x}Al_xN$ coatings, while still showing a single fcc phase.

It was demonstrated that these single-phase films with high Al fractions are enabled by a characteristic microstructure consisting of comparatively large grains with alternating Ti-rich and Al-rich fcc nanolamellae. By using in situ high-temperature synchrotron X-ray diffraction, the sequence of spinodal decomposition and the fcc → wurtzite phase transformation were investigated up to a maximum temperature of 1250°C. Dr. Tkadletz showed that at 1000°C the spinodal decomposition of only the Ti-rich lamellae is observed, while at 1200°C the microstructure shows a complete decomposition and transformation of the coating into a wurtzite AlN matrix containing fcc-TiN precipitates. Above 1200°C a coarsening of the grains can be observed. These in-depth findings regarding the decomposition behavior of CVD-$Ti_{0.2}Al_{0.8}N$ coatings are especially interesting for the mechanical model of SFB-TR 87.

Lena Patterer, project A3 of the SFB-TR 87

Durability of Physical Vapor Deposited CrN-based Coatings

Assistant Prof. Helmut Riedl-Tragenreif from the Technical University of Vienna gave a two-part workshop on 16 December 2021 via Zoom. Prof. Riedl-Tragenreif heads the Christian Doppler Laboratory for Surface Engineering of High-Performance Components and is a group leader at the Institute of Materials Science and Technology at TU Wien.

In the first part 'Durability of physical vapor deposited CrN based coatings - insights on fracture and fatigue mechanisms' Prof. Riedl-Tragenreif focused on mechanical testing of coating materials with respect to thermo-mechanical fatigue which is for example relevant for coated turbine blades. In the beginning different testing scenarios, such as beam bending of free-standing coatings, coating-substrate interface analyses as well as tests of coatings including the substrate were reviewed. Cr and CrN coatings were used as model systems for fatigue testing and while the elastic modulus was 300 GPa for both material systems, the fracture toughness K_{IC} of Cr was approximately two times higher than for CrN. Cyclic bending of pre-notched, unstrained micro-cantilever beams revealed either stable testing conditions (when the force was below the critical breakdown force) or immediate critical failure. No signs of fatigue up to the regime close to the fracture force were observed by in situ X-ray diffraction characterization during fatigue testing. Hence, it can be concluded that these coating materials behave as bulk ceramics and the fatigue resistance is solely governed by the K_{IC} limit. These insights were especially interesting for the mechanical model of SFB-TR 87.

The second part 'Ternary transition metal diborides: A new generation of protective coating materials?' was an overview of recent developments in the framework of protective diboride coatings. Prof. Riedl-Tragenreif discussed the issues of brittle material behavior as well as the formation of volatile oxides during annealing in air and presented studies of diborides based on the hexagonal AlB_2 prototype structure. Strain maps of WB_x based on fast Fourier transformations revealed highly-defective regions and it was found that the AlB_2 structure is more stable for understoichiometric $WB_{1.5}$. Hence, this structure is stabilized by boron defects. Due to the inherent anisotropy of this material, (0001)-oriented coatings exhibited superhardness (≥ 40 GPa), however, the thermal stability is limited as annealing at 600°C for 10 minutes in air caused the formation of a large oxide scale. Ta-alloying enhances the thermal stability above 1200°C, while the oxidation resistance is still limited. Enhancement of the oxidation resistance can be achieved by Si additions. For example Ti-Si-B, Cr-Si-B and Hf-Si-B showed extremely low oxidation rates. In turn, a drop in hardness from 50 to 30 GPa was observed, when 15 at.% of Si were added. These insights are interesting for both the mechanical as well as the plasma surface model of SFB-TR 87.

Marcus Hans, project A3 of the SFB-TR 87

Summit meeting of the SFB-TR 87

In order to bring the findings of the last twelve years to a round conclusion, a summit meeting was organized by Peter Awakowicz, the spokesperson of the SFB-TR 87. This took place from May 15 to May 18 in the conference center at the Eibsee. Moreover, the Mercator Fellows Prof. Dr. Ludvik Martinu, Prof. Dr. Christian Mitterer as well as the guests Prof. Dr. André Anders and Hon.-Prof. Dr. Christian Oehr were included in the program. Their lectures were the highlights of the lecture series.

Furthermore, the most important results of the individual research areas were presented in lectures. In addition, junior researchers were asked to give comprehensive presentations in groups. The fruitful discussion within the research-oriented sessions as wells as over a cup of coffee were a great successful of this event.

In the end, the presentation on new research questions by Peter Awakowicz could motivate the future research fields very nicely. Thanks to Peter Awakowicz, it is his credit through his communicative way to bring together the different researchers over twelve years and to lead them to high class results. In addition, many young researchers have been trained during this time and have been very well supported in the consortium.

Marina Prenzel, public relations of the SFB-TR 87 & CRC 1316

UPCOMING DATES

SPB-TR 87:

22. JUN

IANiS workshop: Future Ideas and Directions:

Online

Possible future research ideas and corresponding collaborations

CRC 1316:

1. JUL

Seminar talk: Prof. Dr. Nader Sadeghi

NB 5/99, Ruhr-University Bochum

Electron density measurements in plasmas

8. JUL

Meta data scheme discussion INP Greifswald:

Online

Emission spectroscopy

12.—13. JUL

Summer Retreat:

Bad Honnef

22. AUG

Plasma Bio working group meeting:

Online

15.—17. NOV

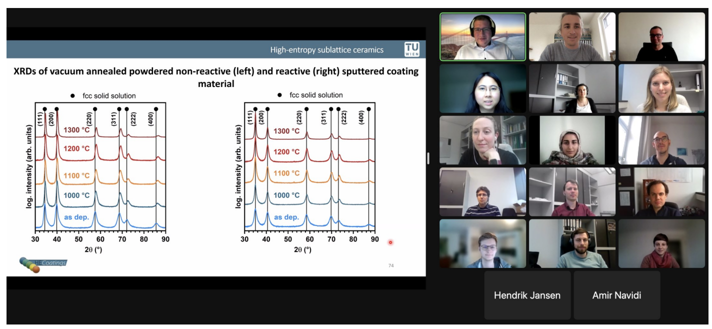
Autumn Project Meeting incl. Workshop with Prof. Dr. Caroline Richter

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

Transition metal nitrides as protective coatings: From TiN to MEN to HESN

Dr. Alexander Kirnbauer from the Technical University of Vienna gave a seminar about nitride coatings on 17 March 2022 via Zoom.

He started with the discussion of binary transition metal nitrides (TMNs) and TiN as well as CrN are prominent nitride material systems. While TiN exhibits softening at annealing temperatures of 400°C, CrN shows significant N-loss above 800°C. Hence, their low thermal stability limits the application in high temperature processes. In order to improve the thermal stability and oxidation resistance, Al has been added. During annealing at high temperature, the age hardening effect can be observed and causes an increase of the hardness. (Ti,Al)N and (Cr,Al)N thus became widely used protective coatings.



Dr. Kirnbauer emphasized that alloying is a viable strategy to tailor the properties of the coatings. Multi-element nitrides (MEN) alloyed with refractory metals such as Ta, Mo, or W and the newly developed concept, high-entropy sublattice nitrides (HESN), by using at least five metals to obtain a configurational entropy larger than 1.5R on the metal sublattice were adopted. The (Hf,Ta,Ti,V,Zr)N system demonstrated a N_2-flow dependent thickness and morphology, while the chemical composition and phase formation were not significantly affected. These coatings were demonstrated to be thermally stable up to 1300°C without secondary phase formation as revealed by atom probe tomography. This strategy opens a new avenue for protective nitride coatings and is relevant for the mechanical model as well as the interaction model of SFB-TR 87.

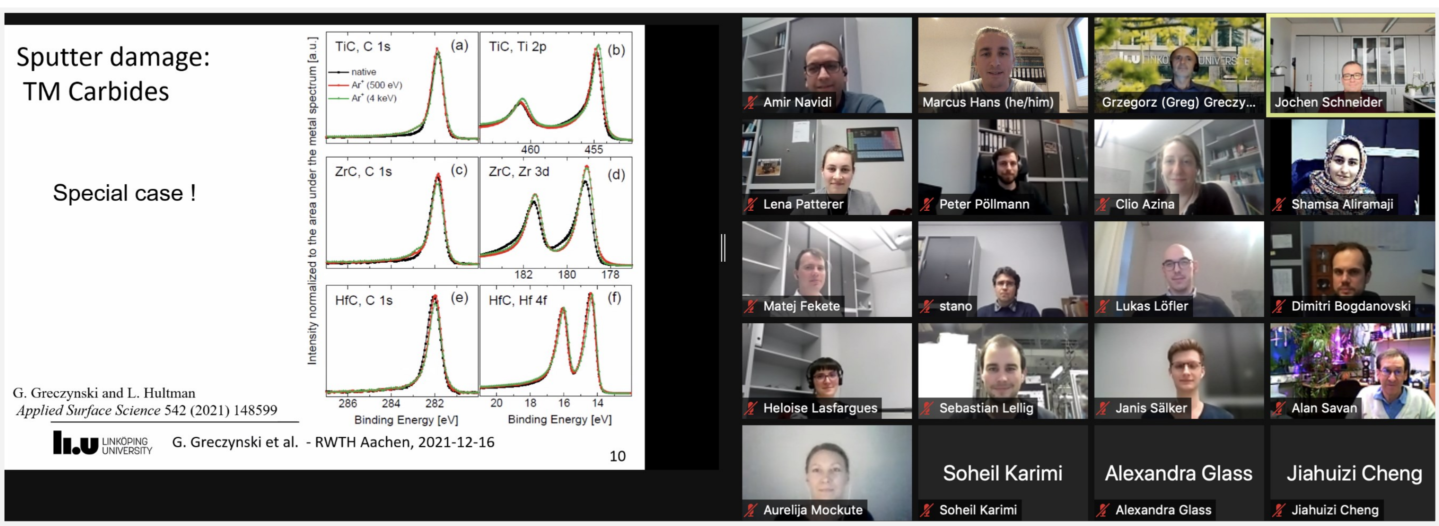
Yu-Ping Chien, project T1 of the SFB-TR 87

Toward Energy-Efficient Physical Vapor Deposition: Routes for Replacing Substrate Heating During Magnetron Sputter Deposition by Employing Metal Ion Irradiation

Prof. Grzegorz Greczynski from Linköping University gave a Zoom workshop on the topic of *Toward energy-efficient physical vapor deposition: routes for replacing substrate heating during magnetron sputter deposition by employing metal ion irradiation* on 16 December 2021. The development of energy-efficient production routes is a relevant topic for thin-film research, especially with respect to climate change.

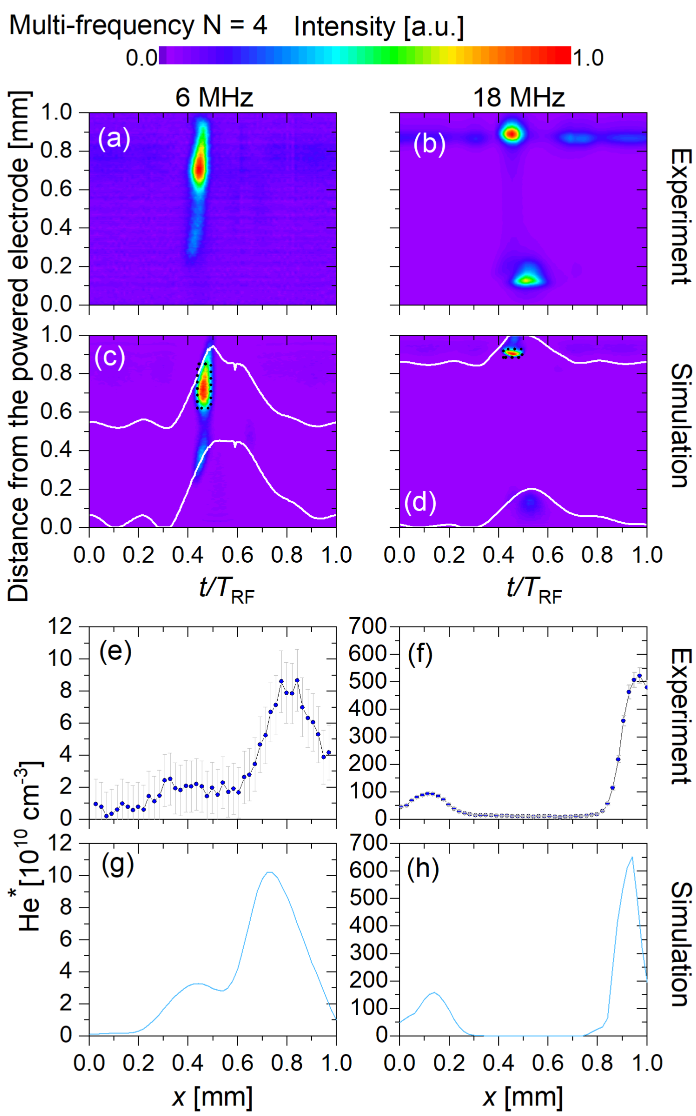
Physical vapor deposition processes often consume significant amounts of energy due to extensive heating of the substrates on the one hand and water cooling of temperature-sensitive components on the other hand. Substrate heating is often needed for higher adatom mobility that guarantees a high-quality fully dense thin film. However, the adatom mobility can also be supplied by effective low-energy recoil creation induced by heavy metal ion irradiation of the growing thin film. Prof. Greczynski showed in his talk examples of metal-ion irradiation by creating Ta^+ and W^+ ions from a HPPMS target while Ti or (Ti,Al) is sputtered by DCMS from a second target, growing dense (Ti,Ta)N, (Ti,Al,Ta)N and (Ti,Al,W)N thin films on a substrate that is biased synchronously. The incoming heavy Ta^+ or W^+ ions initiate low-energy recoils of the lighter atoms which are the dominant components of the DCMS-grown thin films. Consequently, a densification of the growing film can be observed with only low concentrations of the heavy elements. By investigating the mechanical properties using nanoindentation, it was shown that (Ti,Al,W)N thin films obtain hardness values comparable to the hardness of (Ti,Al)N grown at 500°C. No external heating is used for this deposition process, requiring ~ 65 % less energy compared to the conventional (Ti,Al)N deposition at 500°C. This means not only a more energy-efficient production route, but it also widens the application window toward temperature-sensitive substrates like polymers. All in all, this workshop gave an interesting insight into an innovative research topic and was of relevance for the plasma-surface, the mechanical, as well as the interaction model of SFB-TR 87.

Lena Patterer, project A3 of the SFB-TR 87



PROCESS CONTROL IN MICRO ATMOSPHERIC PRESSURE RF PLASMA JETS BY VOLTAGE WAVEFORM TAILORING AND CUSTOMIZED BOUNDARY SURFACES

The recently published paper in project A4: "The effects of the driving frequencies on micro atmospheric pressure He/N_2 plasma jets driven by tailored voltage waveforms" (J. Phys. D: Appl. Phys. 55 (2021) 095204) acts as a direct follow up to previous work. Previous works "Control of electron dynamics, radical and metastable species generation in atmospheric pressure RF plasma jets by Voltage Waveform Tailoring", Plasma Sources Sci. Technol. **28**, 094001 (2019), and "Helium metastable species generation in atmospheric pressure RF plasma jets driven by tailored voltage waveforms in mixtures of He and N_2", J. Phys. D: Appl. Phys. **53**, 185201 (2020), have successfully shown that Voltage Waveform Tailoring (VWT) in high pressure discharges provides an opportunity to control and enhance the generation of different excited/reactive species. The main motivation behind this work is to extend the results of earlier publications by combining VWT and variation of the base frequency to further enhance the control over the generation of different excited/reactive species. Such species are important for a great variety of applications such as, sterilization, virus/bacteria deactivation, cancer treatment etc.



In collaboration with our Mercator fellow Zoltán Donkó and based on a combination of experiments (COST-Jet with phase resolved optical emission spectroscopy (PROES), tunable diode laser absorption spectrsocopy (TDLAS)) and PIC/MCC simulations, we found that the combination of VWT and a variation of the base frequency has an additional influence on the asymmetry in electron impact excitation and helium metastable density distribution troughout the discharge gap when compared to VWT alone. Here the asymmetry is reduced at lower base frequencies of 6 MHz with four consecutive harmonics (Fig.1 (a), (c)) or strengthend at higher base frequencies of 18 MHz with four consecutive harmonics (Fig.1 (b), (d)) compared to the standard case at 13.56 MHz presented in earlier works for the He/N_2 mixtures. Both simulations and experiments show that a higher base frequency leads to a narrowing of the area of high electron impact excitation during the sheath collapse, which is also reflected in the up to two orders of magnitude higher and spatially more focused helium metastable density distribution, see Fig.1 (e), (g) and Fig.1 (f), (h). The experimental results for the helium

Figure 1: Normalized spatio-temporal plots of the electron impact excitation rate obtained experimentally (a) - (b) and from PIC/MCC simulations (c) - (d), for "valleys"- voltage waveforms consisting of four harmonics (N=4) base frequencies 6 MHz and 18 MHz. Spatial resolved time averaged helium metastable density profiles obtained experimentally (e) - (f) and computationally (g) - (f) for the same conditions. He flow: 1000 sccm, N_2 concentration: 0.1%, Vpp = 500 V.

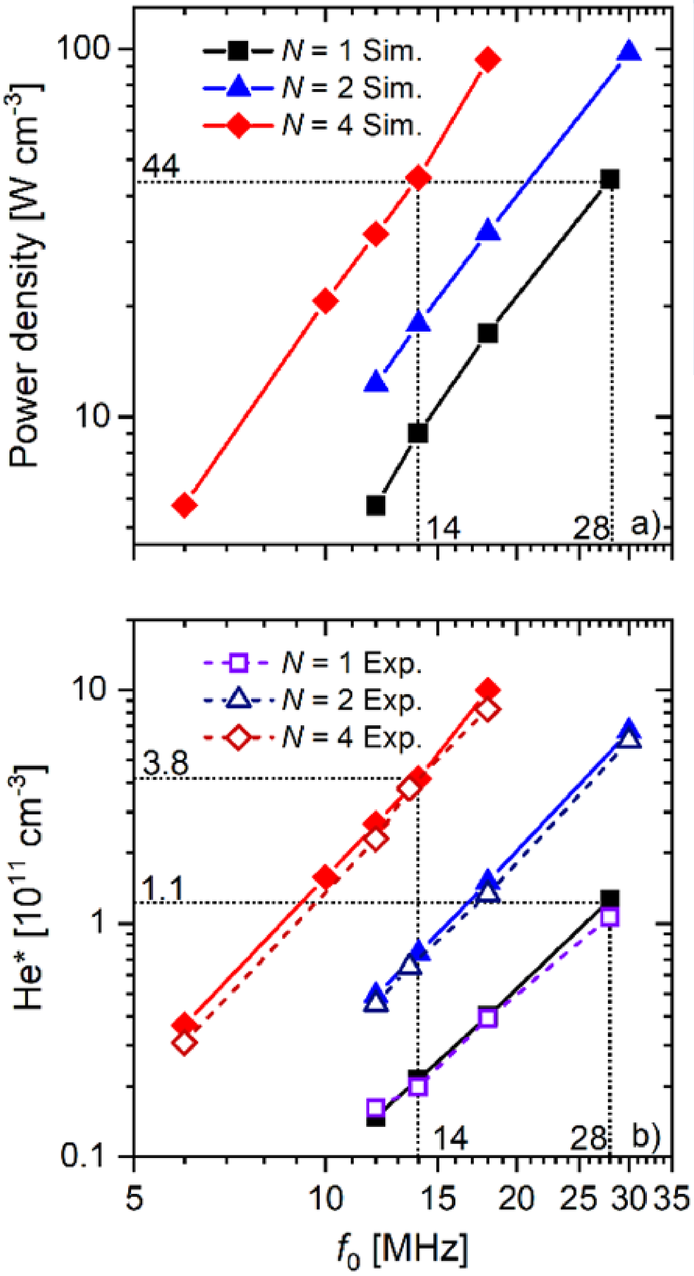


Figure 2: Computed power density dissipated in the plasma (a). Computed and experimentally obtained space- and time-averaged helium metastable density (b). for different fundamental driving frequencies and numbers of consecutive harmonics, N. The vertical dashed lines indicate exemplary (fundamental) driving frequencies (f_0) for the single- and multi-frequency VWT scenarios at which the same power density is dissipated in the plasma. He flow: 1000 sccm, N_2 concentration: 0.1%, Vpp = 500 V.

metastable densities were obtained in a collaboration between the projects A4 and B2. To further clarify and compare the effects of varying the base frequency in combination with VWT to VWT alone, the power density was computed for different base frequencies and different numbers of consecutive harmonics ranging from one to four, Fig.2 (a). Furthermore, the calculated helium metastable density was found to be in good agreement with experimental data, see Fig.2 (b). These results further prove the superior efficiency of VWT for generating such species as compared to classical single frequency operation and the broad range of control that can be obtained over plasma internal parameters with this method.

Overall, the results showed that the variation of the base frequency in combination with VWT allows us to control the electron driven plasma chemistry in a broader range when compared to earlier work and to access regimes that were not possible to achieve with a single frequency operational mode. This is highly relevant for numerous biological and technological applications.

Gerrit Hübner, project A4 of the CRC 1316

Maximilian Klich wins prize for Master thesis

During the annual faculty celebration of the Faculty of Electrical Engineering and Information Technology, Maximilian Klich received the Faculty Award for his 2021 Master's thesis entitled "Ion Dynamics in Capacitively Coupled Argon-Xenon Discharges" made possible by the TopING program. The award ceremony was held on 3/6/22 during the ETIT Faculty Academic Annual Celebration.

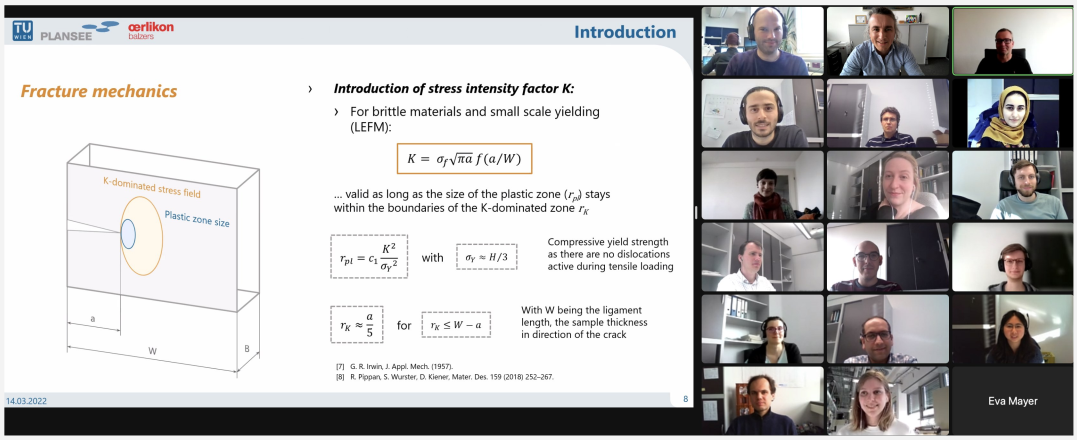
His work was done in the framework of project A8 of the CRC 1316. Finally, the results of his master thesis could already be written down in a publication, see M. Klich et al., *Plasma Sources Sci. Technol.* **30**, 065019 (2021).

Congratulations on winning the award!

Marina Prenzel, Public Relations of the SFB-TR 87 & SFB 1316

Fracture Properties of CrN Hard Coatings: Influence of the Microstructure, Alloying Elements and Coating Architecture

Dr. Rainer Hahn from the Technical University of Vienna gave a two-part workshop on 14 March 2022 via Zoom. Dr. Hahn is Post Doc at the Christian Doppler Laboratory for Surface Engineering of high-performance Components and an expert for fracture mechanics.



In the first part 'Theory and Testing Methods' he emphasized that new coating systems need to exhibit outstanding damage tolerance in order to increase the life time of tools and components such as turbine blades or automotive parts. The evaluation of damage tolerance is focused on two major failure modes which are surface cracking as well as interfacial cracking/delamination. Dr. Hahn investigates the failure mechanisms by in situ testing methods such as microcantilever bending and pillar splitting or ex situ cube corner indentations. He covered basic fracture mechanics theory with the Griffith criterion which states that pre-existing flaws in materials can explain differences between the theoretical strength and the necessary stress for fracture of a material as well as the stress-intensity factor which has been introduced by Irwin. Moreover, Dr. Hahn emphasized that linear elastic fracture mechanics is only valid under certain circumstances and discussed cantilever fabrication, necessary geometries as well as all possible sources of errors.

In the second part of the seminar the effect of microstructure, alloying elements and coating architecture were discussed for CrN-based systems. Morphological variations were investigated for cathodic arc-evaporated CrN coatings. Within two experimental series the substrate temperature as well as the substrate bias potential were varied. Evaluation of the hardness by nanoindentation together with structural analysis by X-ray diffraction revealed that the hardness was enhanced with an increasing defect density. The defect density was indicated by the full width at half maximum of diffraction peaks which is affected also by the column width. However, no influence of defect density or column width on the intrinsic material toughness was found. Si additions to CrN resulted in fracture toughness variations and a maximum for optimum Si content. Since the elastic modulus of the CrN coatings was apparently unaffected by the Si content, it could be concluded that the fracture toughness is governed by the grain boundary cohesive energy.

Finally, Dr. Hahn presented TiN/CrN superlattice architectures which were synthesized by magnetron sputtering as well as cathodic arc evaporation. Variations of the bilayer period were done and hardness as well as fracture toughness enhancement were obtained at a bilayer period of 6 nm. Density functional theory calculations were used to show that a maximum in coherency stresses occurs directly at the interface and the cleavage energies of TiN/CrN superlattices were always higher than for monolithic systems. Thus, superlattices enhance both hardness and fracture toughness for similar bilayer periods. These findings are relevant for the mechanical model of SFB-TR 87.

Marcus Hans, project A3 of the SFB-TR 87

Competition between Plasticity and Brittleness in Refractory Ceramics

Prof. Davide Sangiovanni from Linköping University presented a seminar on 'Competition between plasticity and brittleness in refractory ceramics' on 19 January 2022 via Zoom. Throughout this workshop, the powerful combination of density functional theory (DFT) calculations, *ab initio* and classical molecular dynamics (AIMD and CMD) simulations in describing the mechanical performance of refractory ceramics was comprehensively discussed.

The talk was focused on the use of DFT calculations to explore the effects of alloying cubic binary nitrides with other transition metals to enhance toughness. It was shown that the toughening mechanism of such ternary systems depends significantly on the valence electron concentration (VEC) as revealed by electronic structure analysis. To this end, the V-Mo-N system showed superior toughness and high-temperature hardness due to the highest VEC amongst the investigated ternary nitrides. These ab initio calculations were then complemented by AIMD simulations to identify atomistic processes and changes in electronic structure which control strength, plasticity, and fracture in $V_{0.5}Mo_{0.5}N$, as well as reference B1 TiN. Tensile deformation of both systems revealed that $V_{0.5}Mo_{0.5}N$ is considerably tougher than TiN due to highly populated d-d metallic-states, which allow for redistribution of mechanical stresses and dissipation of the accumulated strain energy by activating local structural transformations. These structural transformations were interestingly also observed in the benchmark $Ti_{1-x}Al_xN$ system revealed by the more realistic CMD simulations. The large scale CMD simulations demonstrated that an increasing Al content in ternary cubic $Ti_{1-x}Al_xN$ promotes local martensitic transformations ahead and behind the crack front which is a ductility enhancement mechanism without any dislocation-induced plasticity. These findings are very interesting for the mechanical model of SFB-TR 87.

Soheil Karimi, project A3 of the SFB-TR 87

Science communication via Twitter & Instagram

What is a plasma anyway? Most people have never heard of physical plasmas, let alone know more about what they are characterised by and what they are used for.

Plasmas have received little attention from the general public. To make the subject area and research from it more present, the CRC 1316 and SFB-TR 87, as members of the RDPCI, are now also represented on Instagram under @plasma_rub and on Twitter under @RDPlasma.

News about current developments in research, personnel additions and departures, projects for students, and interesting background knowledge are shared via this.

Instagram: @plasma_rub
Twitter: @RDPlasma

Social media offers the chance to reach a large target group and transport information in a compact and descriptive format, so that the field of plasma physics is carried further outwards.

Maike Kai, public relations for the SFB-TR 87 & CRC 1316

New Scientists within the SFB-TR 87 & CRC 1316

Pia-Victoria Pottkämper studied medical physics at the Technische Universität Dortmund. She wrote her master thesis at the chair for exerimental physics II of the Ruhr-Universität Bochum in the project PlasNOW where she investigated the influence of the humid-

Sabrina Klopsch studied biology with a focus on biotechnology at the Ruhr University in Bochum. Since her bachelor thesis in 2019, she has been working on the B8 project in the CRC 1316 and dealt with the production and characterization of different enzymes and their potential for the application in plasma-driven biocatalysis.

In March 2022, she has re-joined CRC 1316 as a PhD student and will take over the biological part of the new interdisciplinary project B11 of the sec-

David Schulenberg studied electrical engineering at the Ruhr University in Bochum. In his master thesis (2020) he measured different plasma parameters in a symmetric capacitively coupled low pressure plasma. The thesis was part of the SFB TR87. After his master's, he continued working in TR87 before moving to 1316 this year. Here, he will work together with Máté Vass in

Simon Kusmierz studied Materials Science at RWTH Aachen University with emphasis on surface technology and construction materials. He worked as a trained materials tester with a strong background in electron microscopy and failure analysis. In his Master Thesis he developed a method to increase the nutrient transport through non-woven polycarbonate urethane-based stent covers by plasma grafting for the treatment of lung cancer patients.

Timothy Oppotsch studied chemistry at the Ruhr University Bochum. In his master thesis, he investigated the plasma-induced removal of trace oxygen at elevated pressure and the influence of pressure on characteristic parameters. The study further focused on the residence time behavior for the reactor setup used in project A7 and the influence of plasma on it. In February 2022, he joined project A7 to continue the work of Niklas Peters in the second funding period of the ity of the operating gas and the surrounding ambient air on a COST Reference Microplasma Jet and its effluent.

In June 2022 she joined the project B7 as a PhD student. The project investigates the reaction chemistry of plasmas in liquids and its influence on surfaces.

ond funding phase. In this project, the rational tuning of plasma and liquid chemistry will be investigated to improve H_2O_2 formation for the biocatalytic conversion. Her focus in this project will be the identification of chemical pathways of H_2O_2 and how these pathways can be controlled and scaled up for the specific requirements of different enzymes in plasma-driven biocatalysis.

project A4, where Máté will do the simulations and David will work on the experimental part. His task is to determine different plasma parameters along the discharge channel of the COST jet to then use the knowledge gained to optimize the production of certain particle species in the jet. In addition, his data will be needed for comparison with the results from Máté's simulation.

Since August 2021 he continues his scientific work at the Institute of Plastics Processing in Industry and Craft in Aachen. He joined the SFB-TR 87 as a PhD student in the project B1. His research in the project B1 will mainly focus on the upscaling and adjustability of plasma processes and thin film properties of PECVD coatings on plastic substrates.

CRC 1316. The project aims at identifying and studying a synergistic effect of plasma and catalysis which shall be exploited for the plasma-catalytic VOC degradation. For this, Timothy will, inter alia, prepare and investigate electrode configurations coated with different catalytic materials. He will also work on coatings for other projects like A3, to continue collaborations.

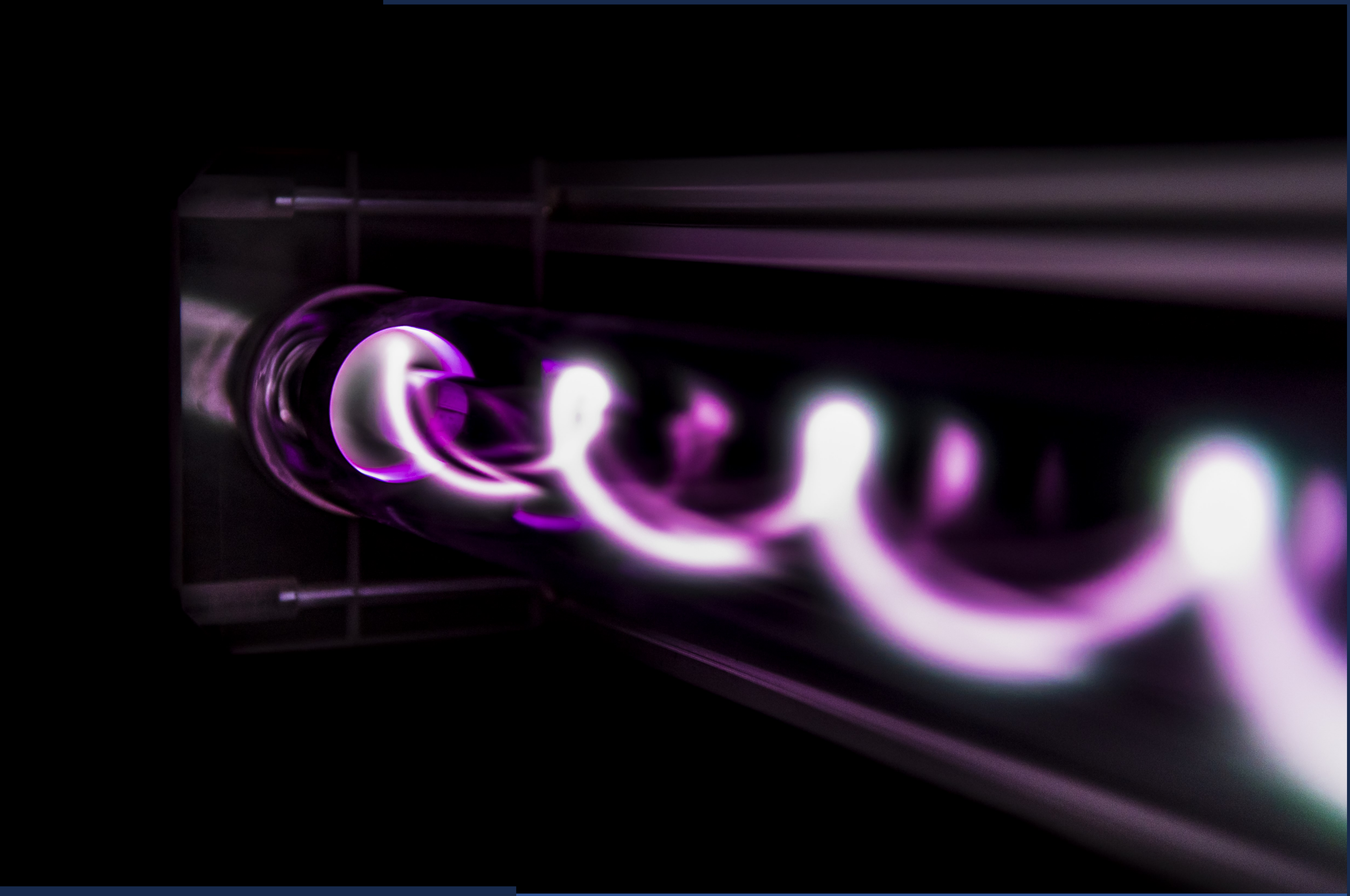
International Workshop on FAIR Data in Plasma Science

On May 16–18, 2022, the project Quality assurance and linking of research data in plasma technology - QPTDat hosted the International Workshop on FAIR Data in Plasma Science online.

The goal of the workshop was to intensify discussions about research data management and data standards in the plasma science community. The contributions ranged from results of the QPTDat project to the presentation of current activities in other projects in the field of plasma science that strive for data and software sustainability, such address LXCat and PlasmaFAIR . Finally, overarching initiatives such as the Open Research Knowledge Graph and the Patents4Science project illustrated how data and information from different sources can be linked together to make them more accessible for science. Finally, the QPTDat infrastructure was outlined as a general approach for trustworthy AI-driven research.

Presenting the structures and recent developments, the CRC 1316 was present with a talk within the event.

Marina Prenzel, project INF of the CRC 1316



IMPRESSUM

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