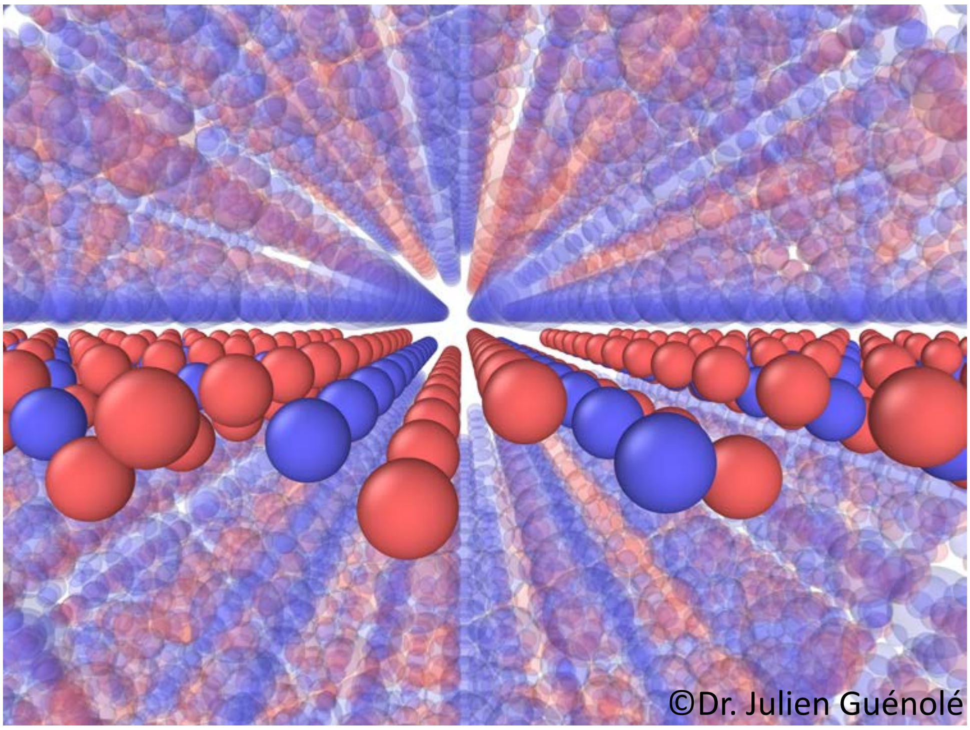
SFB-TR 87

SFB 1316

NEWSLETTER

EDITION 8



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Foreword

Half-time of both collaborative research centres

Next year will be the half-time of the first funding period of the CRC 1316 and of the third funding period of the SFB-TR 87. The activities in both collaborative research centres are highlighted byin several research activity reports, but also more specifically by the collaborations between different research groups – also located at different universities.

Furthermore, many regular meetings are organized that foster the exchange between the members and guests of the research consortia. Both consortia share the training events on scientific methods and on transferable skills. These events are also open for all PhDs interested in plasma science. For example, an excursion to London for ten PhD students was organized at the beginning of 2019 to improve the English skills of early career researchers. This will be repeated in the beginning of 2020.

So called working groups of both collaborative research centres have a special role to stimulate the interaction between the different researchers This is illustrated by interviews with working group leaders from the SFB-TR 87 as well as CRC 1316.

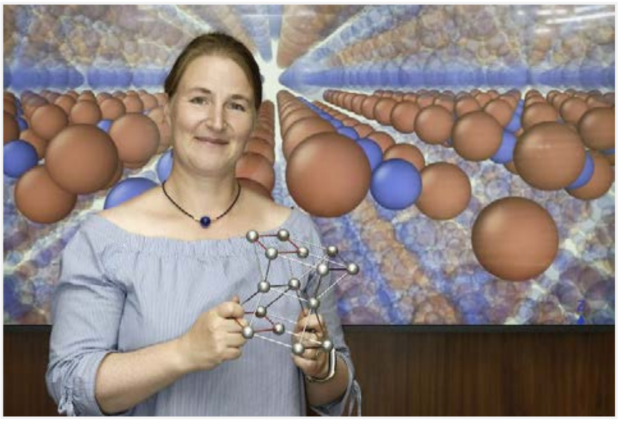
A special highlight in 2019 is the ERC starting grant Prof. Korte-Kerzel PI in the SFb TR 87 on "Fundamental Building Blocks - Understanding plasticity in complex crystals based on their simplest intergrown units".

Finally, the PIs Prof. Mussenbrock and Dr. Trieschmann organized the national conference PT19 in Cottbus this summer, which was a great success and a great platform to disseminate the research outcome in the research centres.

SFB-TR 87

ERC starting grant for Prof. Korte-Kerzel

Prof. Sandra Korte-Kerzel from RWTH Aachen (project A7, SFB-TR 87) has been awarded for a starting grant of the European Research Council. The project of Prof. Korte-Kerzel has the title "Fundamental Building Blocks - Understanding plasticity in complex crystals based on their simplest, intergrown units".



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In detail, new structural materials with high strength and temperature resistance are key to the realization of sustainable energy conversion and mobility technologies. The central question is how to find high-performance materials that combine high strength with the formability essential for safety.

The Starting Grant now makes it possible to investigate the fundamental building blocks of complex crystals. Using mechanical experiments on the nanometer and micrometer scale and high-resolution electron microscopy, the missing fundamental mechanisms and signatures of the plastic deformation of complex intermetallic materials will be investigated. A new approach will be pursued by looking at the fundamental, smaller building blocks instead of the complex large crystal structures of the intermetallic compounds. In this way, it is possible to extend the knowledge about the relationships between crystal structure and properties beyond those of the much simpler metallic crystals. This enables a knowledge-based search for new structural materials.

Marina Prenzel, public relations

Recent research activities – project A3 of the CRC 1316

Excitation and dissociation of CO_2 heavily diluted in noble gas atmospheric pressure plasmas

The excitation and dissociation of CO_2 admixed to argon and helium atmospheric pressure radio frequency plasmas is analyzed. The absorbed plasma power is determined by voltage and current probe measurements and the excitation and dissociation of CO_2 and CO by transmission mode Fourier-transform infrared spectroscopy (FTIR). It is shown that the vibrational temperatures of CO_2 and CO are significantly higher in an argon compared to a helium plasma. The rotational temperatures remain in both cases close to room temperature.

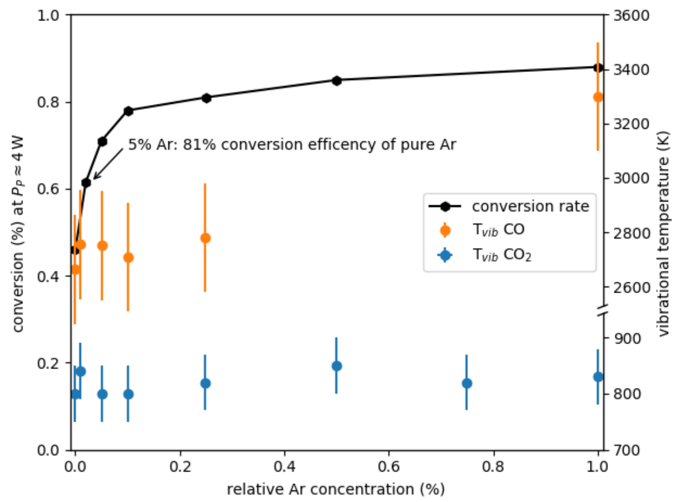


Figure 1: *CO_2 conversion (black, left axes) and vibrational temperatures of CO and CO_2 (orange and blue, right axes) versus argon percentage in helium for a CO_2 admixture of 0.125% and 4 W plasma power.*

The conversion efficiency for the production of CO from CO_2 dissociation, expressed as a critical plasma power to reach almost complete depletion, is four times higher in the argon case (see figure 1). At 5% Ar admixture, already 81% conversion efficiency is reached. This is explained by the lower threshold for the generation of energetic particles (electrons or metastables) in argon as the main reactive collision partner, promoting excitation and dissociation of CO_2, by the less efficient quenching of vibrational excited states of CO and CO_2 by argon compared to helium and by a possible contribution of more energetic electrons in an argon plasma compared to helium.

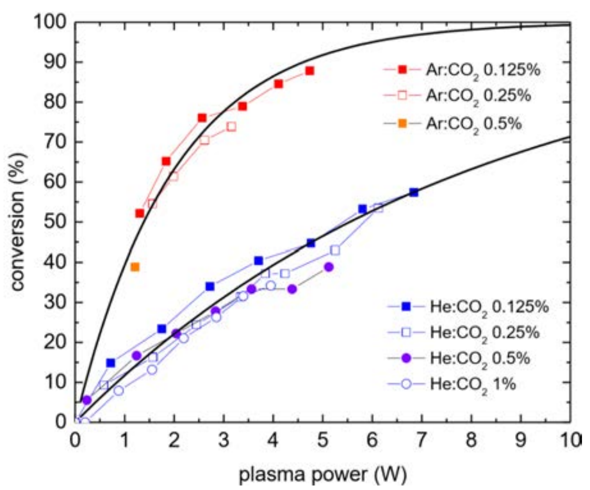


Figure 2: *Conversion efficiency in an argon (red) or helium (blue) noble gas plasma as a function of the plasma power and for varying CO_2 admixture percentages. The solid lines depict a model of the conversion efficiency assuming a gas dominated process and utilizing the concept of a critical plasma power, denoting to the power necessary to deplete CO_2 to its 1/e-th part.*

For CO_2 added to helium-argon-mixture plasmas it can be shown that a very small fraction of argon within a helium plasma already changes the dissociation characteristic towards an argon typical discharge. However, the vibrational temperatures of CO and CO_2 remain unchanged hinting against vibrational pumping of CO_2 prior to dissociation.

The conversion efficiency with increasing plasma power is shown in figure 2. The critical plasma power for helium $P_{crit,He} = 8$ W is four times higher as for argon $P_{crit,Ar} = 2$ W, hence describing a less efficient reaction.

The paper is submitted in *Journal of Physics D: Applied Physics* with the title "Excitation and dissociation of CO2 heavily diluted in noble gas atmospheric pressure plasmas".

Christoph Stewig, project A3 of the CRC 1316

Application of artificial neural networks for the prediction of interface mechanics: a study on grain boundary constitutive behavior

The macroscopic response of materials is rooted in its discrete nature at the atomic scale. For example, the evolution of point defects (e.g. vacancies), line defects (e.g. dislocations), surface defects (e.g. GBs) and volumetric defects (e.g. precipitates) leads to the macroscopic behavior. Evolution of each of these is controlled by motion and interaction of the atoms. Thus, atomistic simulations are proven to be an effective approach to obtain deeper insight into the behavior of a different range of materials.

The complexities of new materials and cumbersome numerical expenses of corresponding material models pose several difficulties for the exploration and simulation of novel material combinations at large scale. Current computational power and novel machine learning (ML) approaches offer scalable methods which can combine insights of material modeling with the flexibility and efficiency of data-driven surrogates. A promising ansatz in multi-scale problems is to incorporate ML models as surrogates for small scale material behavior in macroscopic simulations.

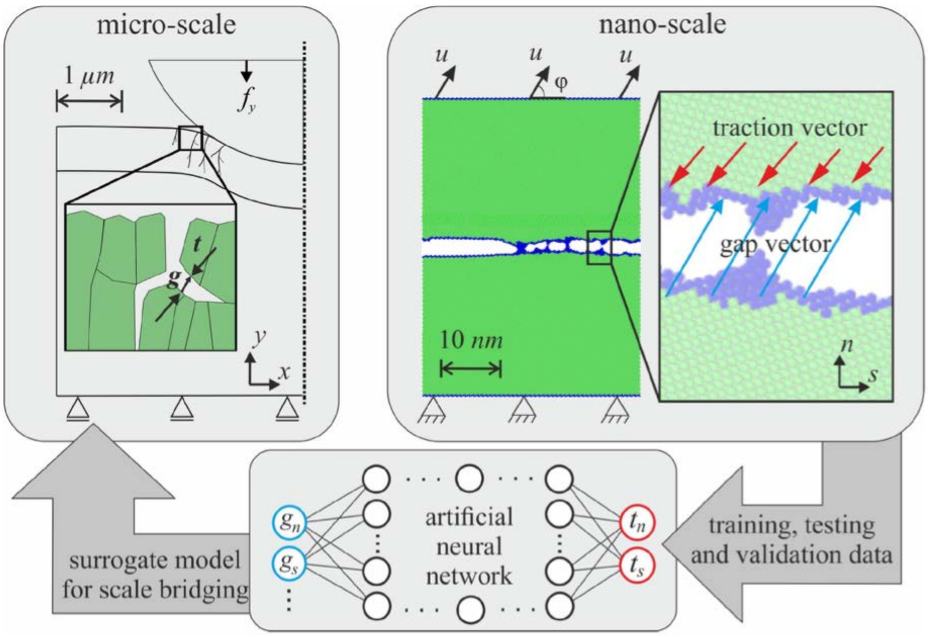


Figure 3: *Scaling bridging utilizing an artificial neural network trained by molecular dynamics simulation results.*

The present work aims at bridging the atomistic scale at GB level and the continuum scale at the polycrystalline level by calibrating an efficient traction-separation surrogate model for the GB, which can then serve for multiscale problems, as illustrated in the figure below. The trained ANN can then serve for large-scale FE-simulation as an alternative to direct MD-FE coupling which is often infeasible in practical applications. Such a strategy and new modeling approach can also be performed based on the DFT calculations or experimental measurements in collaboration with other subprojects in the SFB. As a result, damage and fracture in the coatings can be modeled in an easier way with high accuracy.

The paper is submitted at *Advanced Modeling and Simulation in Engineering Sciences* with the title "Application of artificial neural networks for the prediction of interface mechanics: a study on grain boundary constitutive behavior."

Shahed Rezaei, project A6 of the SFB-TR 87

Research seminars

Several Research seminars embedded into the SFB-TR 87 at MCh in Aachen

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

Diamond-based multimaterials for thermal management applications & on the development of Zr-based MAX phase coatings

Dr. Clio Azina from the Thin Film Physics division at Linköping University presented a two-part lecture on June 17th, 2019. The first part was entitled "Diamond-based multimaterials for thermal management applications" and focused on diamond films grown by laser-assisted combustion flame chemical vapor deposition on C-reinforced Cu substrates. Thermal management is enabled by such a material design since the diamond film is used to spread the heat, while the metal matrix composite substrate acts as heat sink. Due to the lack of chemical affinity between Cu and C, alloying elements such as Ti were utilized in order to form TiC_x carbides which enhance the thermal efficiency. In the second part "On the development of Zr-based MAX phase coatings", Dr. Azina focused on $(Ti_{1-x}Zr_x)_{n+1}AlC_n$ MAX phases synthesized by magnetron sputtering from elemental and compound targets. Utilization of compound targets resulted in the MAX phase formation and employment of elemental targets enabled control over the deposition fluxes. These findings were very interesting for the transfer project T1 within the SFB-TR 87.

Cross-sectional Characterization of Hard Coatings

Prof. Jozef Keckes from Montanuniversität Leoben gave a seminar on "Cross-sectional Characterization of Hard Coatings" on October 2nd, 2019. The first part of the talk was dedicated to utilization of cross-sectional position-resolved X-ray nanodiffraction as a powerful method to characterize the depth evolution of microstructure, texture and residual stress across single- and multilayer coatings with a resolution down to 50 nm (nanobeam size). Within the example of an $Al_xCr_{1-x}N$ multilayer comprising of alternating cubic and hexagonal structures, this technique has revealed high resolution characteristics regarding the phase (de)stabilization and stress evolution in each sublayer. Interestingly, although the stress state of the cubic phase was nearly independent of sublayer thickness, a significant dependence throughout the hexagonal sublayers was identified due to a change from random to preferred orientation. Prof. Keckes continued in the second part talking about a peculiar self-assembled cubic nanolamellae in the TiN/AlN system. Here, the epitaxial self-stabilization of the layers grown by low pressure chemical vapor deposition has been achieved by N deficiency/excess in the layers. In order to obtain tough but still hard coatings, by just two variants of gaseous precursors and through bottom-up self-assembly, an irregularly arranged hard (columnar) and tough (globular) multilayer stack can be formed which exhibits remarkable mechanical properties. The as mentioned method and findings related to this seminar are profoundly in line with the scope of mechanical model within the third phase of SFB-TR 87.

Spokes behavior in both non-reactive and reactive HiPIMS

On October 9th, 2019, a workshop on the characterization of HPPMS plasmas was organized with three contributions from the group of **Prof. Petr Vašina** from the Department of Physical Electronics at Masaryk University. Dr. Peter Klein presented "Spokes behaviour in both non-reactive and reactive HiPIMS" and discussed the classification of spoke types by using a novel characterization method combining strip probes together with fast camera screening. While the strip probes are embedded into the target and locally monitor the current during the whole pulse, the plasma emission was captured with the fast camera. A phenomenological model based on metal resputtering was suggested in order to explain spoke merging and splitting events. Matej Fekete discussed standard and multi-pulse HPPMS in his talk "Ground state number density determination in sputter deposition plasmas by OES" and method of using effective branching fractions to determine the ground state density from self-absorbed spectral lines was introduced. It was shown that the ionization fraction increases with higher reactive gas partial pressure and explained by the discharge current evolution as well as the electron distribution function. Finally, Dr. Jaroslav Hnilica presented "Time-resolved imaging of sputtered particles in HiPIMS discharge" and investigated the effect of plasma parameter variations on the dynamics of ground state Ti as well as Ti+ with laser-induced fluorescence combined with atomic absorption spectroscopy. In case of multi-pulse HPPMS an optimum pulse number for enhanced ionization control was suggested and related to the synchronization between ion waves propagating from the cathode and the subsequent pulses. All of the presentations were highly relevant for the plasma surface model within SFB-TR 87 and fostered exciting and stimulating discussions among the participants.

Marcus Hans and Soheil Karimi, projects A3 & T1 of SFB-TR 87

New members

New PhD student within the SFB-TR 87

Xiaofan Xie studied chemistry at the University of Paderborn. In the context of her Master thesis, she worked on the interface analysis of polymer-films and plasma technology. Since October 2019, she is a PhD student within project B3 of the SFB-TR 87.

At the Chair of Technical and Macromolecular Chemistry, she focuses both on the investigation of the formation of membranes by means of plasma chemistry and on the interfacial analysis of the transport and adsorption of molecules on the coated membranes.

Her work is integrated in the concept of project B3 to investigate the adhesion mechanisms, permeability and extensibility of nanostructured plasma coatings on polymer substrates.

New Postdoc and research assistant within the CRC 1316

Hyo Sang Jeon has received his doctorate degree from the University of Science and Technology (UST) in Korea. During his Ph.D., his research topic was "solar-fuel technique" to convert the solar energy to useful chemical fuels.

Since September of this year, he is working as a Postdoc within project B1 at FHI Berlin, which focuses on the investigation of plasma induced nano-structuring for catalyst activation under operando conditions.

In this project, his main work is the synthesis of active catalysts by using plasmas and the analysis of the electrochemical catalytic performance through the operando characterisations.

Tim Dirks studied biology at the Ruhr-University Bochum. In the field of applied microbiology, he already worked in the with plasmas during his Bachelor thesis on the impact of protein overproduction in bacteria on their survival of plasma treatments. His Master thesis on the plasma-induced activation of Hsp33 bacteria was associated with the CRC 1316.

Since November 2019, he is working as a research assistant on project B8 which focuses on the investigation of new concepts of the combination of biocatalysis and plasmas.

The focus of his work lies on the investigation whether Hsp33 bacteria show a protein-protecting effect in the course of plasma-driven biocatalysis. In addition, he is continuing his research on the plasma-induced activation of Hsp33.

New Administrative Assistance for the CRC 1316

Since November of this year, **Annika Kieren** is working as a managing assistant for the CRC 1316 and is responsible for the administrative work. She will be managing both office communication and third party funding.

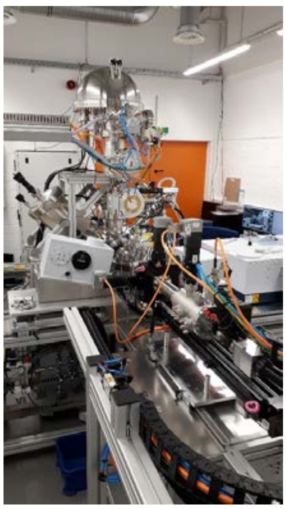
Annika Kieren is the contact person for all questions within the CRC 1316 concerning financial or activity responses.

For clarifcation of administrative questions, please write to annika.kieren@rub.de or sfb1316@rub.de. You can also reach her under the telephone number 0234-32-23672.

New experiment – project B3 of the SFB-TR 87

SFB-TR 87 receives new Near Ambient Pressure XPS-IRRAS system

At the Technical and Macromolecular Chemistry department in Paderborn we have a new setup that combines the techniques of near ambient pressure x-ray photoelectron spectroscopy (NAP-XPS) and infrared reflection-absorption spectroscopy (IRRAS).



The setup allows consecutive IRRAS and XPS measurements under identical conditions of pressure (up to 20 mbar) and temperature (from liquid nitrogen, up to 1000 °C). Additionally, there is the possibility to perform XPS characterization of electrochemical processes using a specially designed EC cell. The setup is implemented within the B3 subproject, where it will be first dedicated to the analysis of surface chemistry and variation of the electronic structure of water molecules in sub-nanometric pores and at interfaces.

Teresa de los Arcos, project B3 of the SFB-TR 87

Interview with the working group coordinators of the SFB-TR 87 and CRC 1316

Working groups consist of Ph.D. students within research projects like the SFB-TR 87 and CRC 1316. Generally, they aim to further the collaboration between different subprojects, using their expertise and support their knowledge exchange. We take a look at the IANiS group of the SFB-TR 87 and the working group "Reaction routes in plasma catalysis and surface interfaces" within the CRC 1316. Therefore, we interviewed the corresponding group supervisors Marcus Hans and Jan Trieschmann of the SFB-TR 87 as well as Niklas Peters and Philipp Grosse from the CRC 1316 to give us some insight into the operation of these different working groups.

Special thanks to all of you for giving this interview.

Interview with the working group coordinators of the SFB-TR 87

Jan and Marcus, would you give us a short description about your scientific career and your place within the SFB-TR 87?

Marcus: *In 2017, I finished my Ph.D. studies, supported by the SFB-TR 87. Since 2018, I am group leader for atom probe tomography at Materials Chemistry of RWTH Aachen University and involved in the projects A3 and T1.*

Jan: *I joined SFB-TR 87 in 2012 as a Ph.D. student within projects C6 and later C8 and finished my Ph.D. in 2017. I became involved as a PI in project C8 since 2018, while also changing scientific environment from Ruhr University Bochum to BTU Cottbus-Senftenberg.*

You two are the supervisors of the IANiS group, which is linked to the SFB-TR 87. Tell us, who is part of this research group and what is its purpose?

Marcus: *The working group IANiS ('Interdisziplinärer Austausch von NachwuchswissenschaftlerInnen im SFB-TR 87') aims at connecting Ph.D. students from different subprojects across the project areas A, B and C. In order to understand the contributions of other projects, knowledge transfer is of paramount importance.*

Jan: *The intention of IANiS is fostering exchange among Ph.D. students. Thus, we established a series of 'Hands-on Workshops' (HoW), where Ph.D. students from the research consortium are invited to join their fellow host Ph.D. students, to assist them in conducting their research methods. It is impressive to see how this helps not only in intensifying personal contacts, but also to widen the perspective on possible collaborations.*

Has the IANiS group contacts to other research projects outside the SFB-TR 87 in which the Ph.D. students can participate?

Marcus: *We are closely collaborating with the working group of CRC 1316 'Transient Atmospheric Pressure Plasmas: from Plasmas to Liquids to Solids' and it is desired that Ph.D. students exchange across these two collaborative research centers.*

Jan: *A perfect example for this are our 'Joint Workshops' that aim at bridging related – but in terms of project collaborations unconnected – research fields. It was an astonishing and important insight for me, how the topic of our joint workshop 'Plasma modeling and simulation' attracted so much interest from both SFB-TR 87 and CRC 1316.*

What is your personal opinion on working in the IANiS group?

Marcus: *For me, being involved in IANiS means that I can learn a lot about the daily work of different subprojects. Of course, organization of e.g. workshops is associated with work, but it pays off in the end by understanding and meeting other researchers.*

Jan: *I couldn't agree more. It is very inspiring to work with the many enthusiastic young researchers and for me the reward is much larger than the investment.*

Could you give us a glimpse of IANiS future? Where is it headed or where would you like to see it?

Marcus: *The idea of connecting project areas A, B and C concerning the HoWs is ongoing and our next step would be aiming for a workshop in the project area B. Moreover, in addition to topical seminars, we want to try different knowledge transfer concepts in the framework of flipped classrooms.*

Interview with the working group leaders of the CRC 1316

After shedding some light on the inner workings of an established group like IANiS, we now take a look at the younger "Reaction routes in plasma catalysis and surface interfaces" group, which is forming just now.

Niklas and Philipp, please tell us about your scientific path and what you do in the CRC 1316.

Niklas: *I have started an apprenticeship as lab assistant before my BA in Recklinghausen in Chemistry. For the MA I switched to Bochum in the Laboratory of Industrial Chemistry. Here I work on heterogeneous catalysts and surface sensitive methods. With the beginning of my Ph.D. I had the first contact with plasmas. In the CRC 1316 I work in the Project A7.*

Philipp: *I am a Ph.D. student in my third year and I work at the Department of Interface Science, on the Fritz Haber Institute (FHI) of the Max Planck Society. Within the scope of project B1, my work involves the benchmarking of catalysts of other projects, providing samples, and development of "in-situ plasma enhanced electrochemistry".*

What is your position in the working group and who is part of it?

Niklas: *We are the organizers or contact persons of the group and inform the researchers from the physic and engineering groups of Bochum and Ulm when the next meeting will take place and try to prepare a small topic for each meeting.*

Philipp: *Our research group consists of people form the physics, chemistry, and engineering departments and we focus on sharing the various in-situ and operando techniques to link effects of the plasma to catalytic performance.*

Because you just begun collaborating in the group, you are currently not settled on its implementation. What is the goal of the research group in your opinion?

Niklas: *I think at the moment it is more an exchange of methods than results, because the researchers need to know the expertise of the different fields. Since we just met two times there is still much to do.*

Philipp: *We use the research group to communicate ideas and develop projects that can corroborate other project's findings as well as sharing the expertise between the Ph.D. students.*

What would you say are the benefits of working within the research group?

Niklas: *For me as a Chemist, I think the frequent exchange with the "real" plasma scientist is fruitful every time. Since there are many different research fields needed in the CRC 1316, it would be impossible to be an expert at every field.*

Philipp: *The thing that sticks out the most to me is sharing expertise. As an example: designing and implementing plasma setups can be challenging for a chemist like me, which, on the other hand, is everyday's work for an engineer or physicist.*

Are there particular challenges for you as organizers in establishing the operation methods within your group?

Niklas: *The most abundant problem at the moment is the choice of good meeting times especially for meeting over video conferences. And I think we as group are still not very clear what we want to do besides expertise exchange.*

Philipp: *Since most groups have just finished laying the groundworks of their respective projects, we have not yet progressed to the stage of actual application of plasmas on catalysts. Therefore, the interest and attendance is a little bit less then desired. Additionally, the large geographical separation of the interested people makes organizing meetings challenging.*

What is your personal opinion on working in the research group and what do you hope to learn?

Niklas: *Besides from the scientific input, I hope to get a better feeling how to work better in such working groups.*

Philipp: *I find the introduction of individual research (sub-)groups a promising addition. It is helpful to discuss topics with peers in a smaller scope and discuss amongst people from similar fields (although with different background).*

Could you give us a glimpse of your working groups future? Where is it headed or were would you like to see it?

Niklas: *I hope after several meetings, the members of the group know exactly who has the expertise in a research field needed and who to ask when they have a particular problem.*

Philipp: *We would like to investigate the mechanisms that make plasma treatment on catalysts desirable and hopefully establish a good and productive interaction with more of the other projects.*

Sascha Chur, public relations

Recent research activities – project A7 of the CRC 1316

Catalytic carbon monoxide oxidation over potassium-doped manganese dioxide nanoparticles synthesized by spray drying

One of the major objectives of the CRC 1316 is the investigation and understanding of the complex interactions between a non-thermal plasma and heterogeneous catalysts. The first results of project A7 describing the thermocatalytic oxidation of CO over MnO_2 catalysts were recently published in *Emission Control Science and Technology*. Particularly, the effect of the incorporated alkali ions on K^+ and Na^+ on the structural properties and the catalytic performance was emphasized to derive structure-activity correlations.

The MnO_2 catalysts were synthesized by a semi-continuous spray drying procedure based on the comproportionation reaction of $Mn(NO_3)_2$ and $KMnO_4$. Solutions of both compounds were continuously mixed in a micromixer and the emerging suspension was rapidly quenched by spray drying to inhibit further particle growth. In order to exchange the K^+ ions by Na^+ ions, $NaMnO_4$ was used instead of $KMnO_4$ during the synthesis. After washing and drying of the catalysts a fine brown powder was obtained, which was used as prepared or calcined at 450 °C or 500 °C for 4 h in synthetic air.

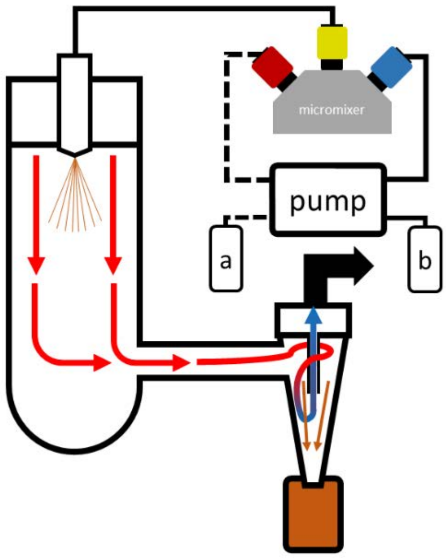


Figure 4: *Schematic illustration of the spray dryer.*

As shown by the XPS results and TPO profiles Mn (IV) is the predominant oxidation state of all samples prior to calcination proving that all catalysts consist of MnO_2. However, the XRD patterns of the uncalcined catalysts reveal an X-ray amorphous structure preventing a more in-depth phase identification. After calcination the phase structure strongly depends on the type and amount of the incorporated alkali ion. The presence of K^+ promotes the formation of crystalline α-MnO_2 and stabilizes its tunnel structure up to temperatures of 500 °C. Lower amounts of K^+ or the exchange with Na^+ lead to less crystalline phases after calcination at 450 °C and to the formation of crystalline α-Mn_2O_3 after calcination at 500 °C.

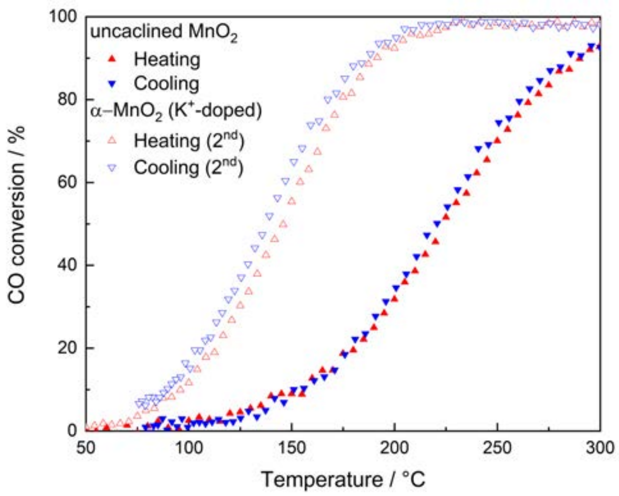


Figure 5: *CO conversion as a function of temperature over uncalcined MnO_2 and K^+-doped α-MnO_2.*

The catalytic CO oxidation was performed in a microreactor set up equipped with a non-dispersive IR detector. All uncalcined catalysts revealed a similar catalytic performance regardless of the type or amount of the incorporated alkali ion. Even though the specific surface area of the catalyst decreased from 77 $m^2\,g^{-1}$ to 37 $m^2\,g^{-1}$ during calcination the pure α-MnO_2 phase exhibited a superior catalytic activity. Over α-MnO_2 the temperature at which full conversion was achieved was shifted towards lower temperatures by more than 100 °C. In contrast the catalyst containing α-Mn_2O_3 show a catalytic activity similar to the uncalcined catalysts indicating that not only the higher degree of crystallinity but also the structural properties of α-MnO_2 cause its high catalytic activity. The incorporation of K^+ ions is required to stabilize the tunnel structure of α-MnO_2.

It was shown that the phase composition of MnO_2 catalysts has a tremendous influence on the catalytic activity. By doping of MnO_2 with K^+ ions the most active phase, α-MnO_2 was stable at temperatures up to 450 °C during catalytic CO oxidation. In future studies the synthesized MnO_2 catalysts will be applied in the plasma-assisted oxidation of volatile organic compounds (VOCs). The electrode configuration of a surface dielectric barrier discharge (SDBD) will be coated with the catalysts to establish a close contact with the discharge volume. It will be exciting to investigate whether the structure-activity correlations derived for thermal catalysis are also valid in plasma catalysis.

Kevin Ollegott, Niklas Peters & Martin Muhler, project A7 of the CRC 1316

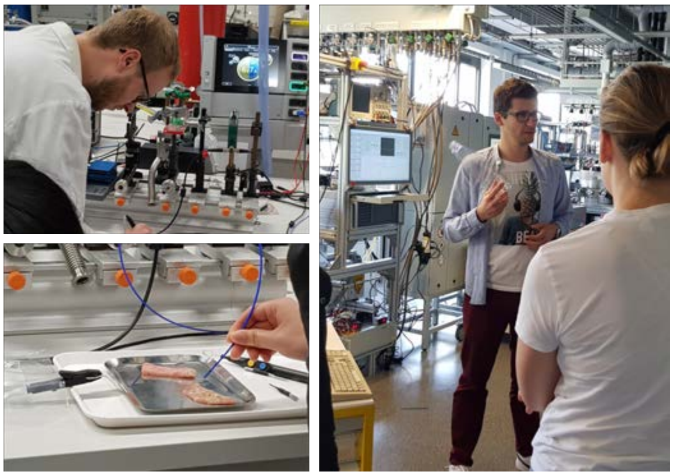
Activities for pupils

AEPT joins Summer Campus at RUB

Between July 15th and July 17th, 2019, the Summer Campus took place the Ruhr-University Bochum. At the Summer Campus, pupils interested in studying get to know the RUB.

The event always takes place during the summer holidays. For pupils who are still unsure which course of studies to choose or would like to get to know the chosen course better, the Summer Campus is the right place.

During the Summer Campus days, the pupils experience the range of faculties and advisory services. Furthermore, they can try out their skills and interests in workshops. Here, the research group of Prof. Awakowicz offered a workshop with the title *Exciting Plasma Technology - Microwave Reactor, Doppe-ICP and more*. Finally, pupils can come in touch with different people, which are also important in their further studies: Teachers, students and student advisors.



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Marina Prenzel, public relations

Conference report

PT19 in Cottbus

The conference which was hosted by BTU Cottbus-Senftenberg started on June 17th, and lasted until June 19th, 2019. The conference was a great success overall. A broad spectrum of different plasma technological applications and basic research was addressed.

Dr. Michael Zeuner (Chemnitz), Dr. Edmund Schüngel (Trübbach) and Prof. André Anders (Leipzig), for example, reported on cathode sputtering (sputtering), which is also used in the SFB-TR 87, and its inherent processes. In addition, Ante Hecimovic (Garching), former member of the SFB-TR 87, reported on his current work (title: *Plasma diagnostics of microwave plasma torches for CO_2 conversion into CO as a raw material for chemical processes*) in an invited lecture.

There were also poster prizes to be won at the PT19. Christoph Stewig (CRC 1316) took the 3rd place (title: Influence of a catalyst on CO_2 dissociation in a non equilibrium atmospheric pressure helium plasma jet)! Moreover, Tobias Gergs from project C8 of the SFB-TR 87 took the 1st place (title: Charge transfer model for reactive molecular dynamics simulations).

Tobias Gergs, project C8 of the SFB-TR 87

Recent research activities – project C1 of the SFB-TR 87

Ion energy control via the Electrical Asymmetry Effect to tune coating properties in reactive radio frequency sputtering

Within the SFB-TR 87, a cooperation between the three sub-projects A3, C2 and C1 resulted in a scientific paper concerning investigations about the plasma-surface-interaction in a large-area multi-frequency capacitively coupled plasma (MFCCP). Tailoring of the plasma-surface-interaction with the possibility to synthesize any kind of coating with preferred electrical or mechanical properties is highly desired for industrial applications. Here, especially the control of a reactive sputtering processes for the deposition of thin films with tailored and reproducible properties is highly requested.

In order to gain a knowledge-based understanding of the interaction processes between the plasma and the growing thin film, investigations regarding the effect of plasma parameter variations on the synthesized coating properties are performed, where only one single parameter needs to be varried, while all other process and plasma parameters have to be unchanged. To reach this goal, plasma engineers as well as material scientists worked together to contribute to the plasma-surface interaction model, which is developed within the SFB-TR87. In detail, they use the electrical asymmetry effect (EAE) to control the ion energy at the grounded substrate electrode, E_{ig}, without an influence on the ion-to-growth flux ratio, Γ_{ig}/Γ_{gr}. As a result, it was possible to nearly decouple both plasma parameters with a combination of changing the relative phase shift, θ, between the two applied consecutive driving harmonics $13.56\ \mathrm{MHz}$ and $27.12\ \mathrm{MHz}$ with an adjustment of their driving voltage amplitudes, $\hat{\phi}_{13}$ and $\hat{\phi}_{27}$.

Measurements of the ion energy distribution function (IEDF), $f(E_{ig})$ and ion flux Γ_{ig} at the center of the grounded substrate electrode are done by a retarding field energy analyzer for a reactive Ar/N_2 (8:1) plasma at 0.5 Pa. The respective growth flux, Γ_{gr}, is proportional to the deposition rate, R_d, which is determined including profilometry, for the case of synthesized Aluminiumnitride films (AlN). The results show, that the mean ion energy at the center of the grounded electrode, E_{ig}^{m}, can be varied within a range of $38\ \mathrm{eV}$ and $81\ \mathrm{eV}$ and correlates with a modification of the analysed film characteristics, while the ion-to-growth flux ratio Γ_{ig}/Γ_{gr} can be kept constant.

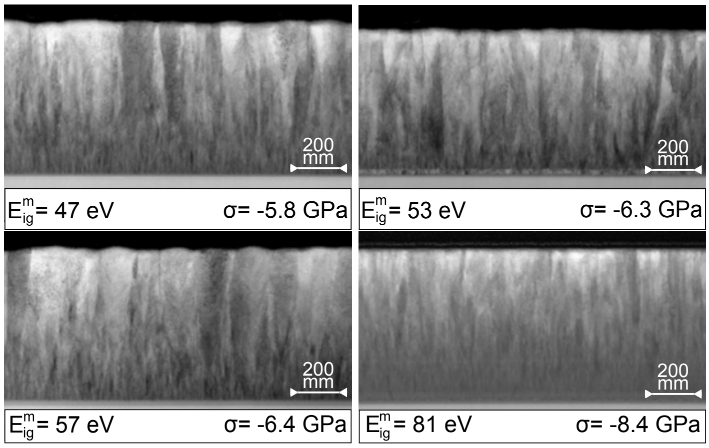


Figure 6: *Measured IEDF at the center of the grounded electrode $f(E_{ig})$ for different θ, while adjusting the driving voltage amplitudes ($\hat{\phi}_{13}/\hat{\phi}_{27} = 2.3\,\forall\,\theta$ at $0.5\ \mathrm{Pa}$ Ar/N_2 (8:1)). Adapted from [1].*

The AlN thin films show an increase in compressive film stress from −5.8 to $-8.4\ \mathrm{GPa}$ as well as an increase in elastic modulus from 175 to $224\ \mathrm{GPa}$ as a function of the mean ion energy (see figure 6). Moreover, XRD measurements reveal a transition from the preferential orientation (002) at low ion energies to the mixed case with (100), (101) and (110) orientations at higher ion energies. Thus, the effects of the ion energy onto the growing films are identified, while other process relevant parameters remain unchanged.

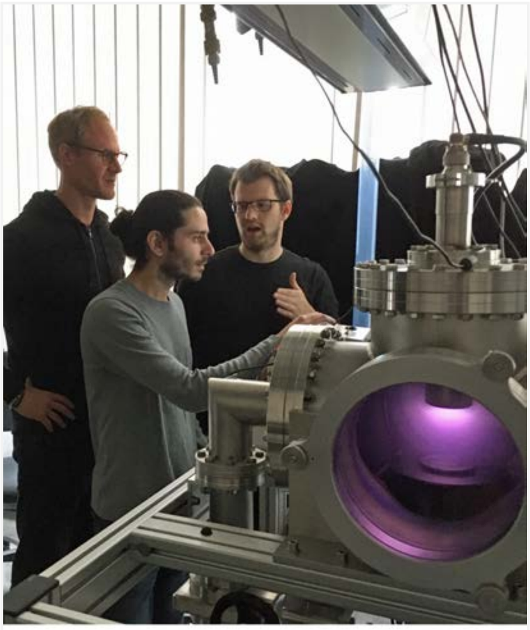
The paper is published in *Plasma Sources Science and Technology*, volume 28, number 114001 ([1] *https://doi.org/10.1088/1361-6595/ab504b*).

Stefan Ries, project C1 of the SFB-TR 87

SFB-TR 87 activities

Hands-on Workshop 02 - "Plasma Diagnostics"

The plasma surface model of SFB-TR 87 correlates global plasma parameters during thin film deposition with coating properties. In order to predict the coupling quantities chemical composition, density, defect structure and residual stress state from global plasma parameters, advanced plasma diagnostic techniques are required.



This topic was covered by the hands-on workshop "Plasma Diagnostics" of the working group IANiS. On October 15th, 2019, PhD students of the consortium visited the laboratories of the Institute for Electrical Engineering and Plasma Technology at Ruhr University Bochum. The workshop started with a short theoretical introduction to the working principle of the instruments retarding field energy analyzer (RFEA), multi pole resonance probe (MRP) as well as phase resolved optical emission spectroscopy (PROES). Afterwards, the PhD students spent several hours in the laboratories and measured ion energy distribution functions of capacitively coupled plasma with the RFEA, studied excitation processes using time-resolved PROES and determined the electron density of a reactive Al/O_2 plasma by the MRP.

Thereby, this hands-on workshop has made another important contribution to the interdisciplinary exchange of young researchers in SFB-TR 87 and the participants benefited from gaining detailed understanding of plasma diagnostics.

Marcus Hans, project A3 & T1 of the SFB-TR 87

2020

Upcoming Dates

March 7th - 8th
SFB-TR 87 Project Area Meeting A & C
Aachen, Germany

March 8th - 13th
DPG Spring Meeting (SAMOP)
Hannover, Germany

March 13th
SFB-TR 87 Project Area Meeting B
Bochum, Germany

April 1st - April 2nd
CRC 1316 - Project Area Meeting
Berlin, Germany

April 26th - May 1st
47th International Conference on Metallurgical Coatings & Thin Films (ICMCTF)
San Diego, California, USA

June 3rd - 5th
Workshop Plasma-wall interaction: including low- and atmospheric plasmas
Kiel, Germany

June 8th - 11th
9th International Workshop and Summer School on Plasma Spectroscopy (IPS.2020)
Greifswald, Germany

June 22nd - 26th
47th European Physical Society Conference on Plasma Physics (EPS2020)
Sitges, Spain

June 22nd - 26th
HIPIMS 2020
Sheffield, United Kingdom

June 29th - July 1st
CRC 1316 General Assembly
Rolduc, The Netherlands

July 15th - 17th
SFB-TR 87 General Assembly
to be announced

Personal reports from the PPPS & ALD conferences

A large group of members of the SFB-TR 87 joined the 19th Conference Atomic Layer Deposition in July in Seattle. Another group represented the SFB-TR 87 at the PPPS in Orlando. Two students, Dennis Engel and David Zanders, report of the conferences.

Report from the PPPS in Orlando

Dennis: We (a small group from the SFB of the TET and the AEPT) visited the PPPS in Orlando. Here all possible topics in the field of plasma research, together with pulsed discharges, were presented. From our side there were four lectures and one poster, which were all very positively received and led to various interesting discussions. We also watched various lectures and took the opportunity to think outside the box, as the conference was very broadly based.

Besides the scientific activities, we used the time in Orlando to look around there and the surrounding area. Mention should be made of the various theme parks (Universial Studios and Disney) as well as the nearby Kennedy Space Center with the surrounding launch pads for the rockets.

Report from the ALD conference in Seattle

David: At the 19th Conference on Atomic Layer Deposition which took place from 21st until 24th July, 2019 in Seattle. On July 23th, in the session "In-Situ Characterization of ALD Processes" I gave a presentation titled "Investigation of PEALD Grown HfO_2 Thin Films via Near Ambient Pressure XPS: Precursor Tuning, Process Design and a New In-situ Examination Approach for Studying Film Surfaces Exposed to Reactive Gases". In this article, the precursor development for hafnium promoted by the SFB-TR 87 was explicitly discussed. In connection with the contributions of Lukas Mai and Nils Boysen (both MGK sponsored - a poster and another presentation), there were numerous opportunities for me and the others to talk to the audience about our work in cooperation with the SFB-TR 87 and it remains from my point of view that this met with an extremely positive response.

The group of Institute for Electrical Engineering and Plasma Technology and the group of the Theoretical Electrical Engineering at the PPPS in Orlando (left) as well as the group of Prof. Devi on the conference site of the ALD conference in Seattle (right).

Dennis Engel, MGK & David Zanders, project B4 of the SFB-TR 87

Impressum

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