NEWSLETTER

EDITION 14— 12/2022

SFB-TR 87

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

Content

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Foreword

This is the last joint issue of the newsletter of the Collaborative Research Centres SFB-TR 87 and CRC 1316. With the end of the year, the era of the SFB-TR 87 comes to an end. Twelve years of research with many bachelor, master, and doctoral degrees are coming to an end. I did my PhD in the SFB-TR 87 during the first funding period and was then able to take over the public relations project. The famous staircase will always remain in my memory. The many trips to Aachen are also unforgettable.

Not only in the area of the SFB-TR 87 there have been many farewells recently. Many PhD students from both SFBs have graduated or are about to graduate. Thus, there have also been some changes in the hallways of the groups in the SFBs. At the Chair of Plasma Physics (EP2) alone, eight people left in the last months or will leave at the end of the year or at the beginning of the next year, respectively.

These changes also affect the public relations project: Maya Krüger has left us as a student assistant, as has Katharina Laake (born Grosse). Katharina was PI of project B7 of CRC 1316 and supported the public relation project on social media. Katharina has greatly enriched the work in project B7 as well as in social media, we are very grateful for her engagement in the last years.

Patrick Preissing &
Katharina Laake
(both leaving from EP2)

We are also happy to have Ida Hülsbusch, Martha Finke, and Sebastian Wilczek as new team members. Ida and Martha are studying physics and have joined the PR team in different ways. Ida supports the project in both, physics didactics and social media. Martha is also involved in social media, but also in the project week. Finally, Sebastian Wilczek, PostDoc of AEPT's B5 project, has joined the team as scientific support. We are happy to have them, welcome!

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

Upcoming Events of the CRC 1316

28 FEB - 02 MAR
MGK colloquium
Location: Ulm

28 FEB - 02 MAR
PI spring meeting
Location: Ulm

01 MAR
Training workshop:
Electrochemistry
Location: Ulm

20 - 24 MAR
Conference:
DPG spring meeting
Location: Dresden

03 - 04 MAY
Workshop:
1st Workshop on FAIR Data in Plasma Science by INP, CAU & RUB
Location: RUB

19 - 21 JUN
CRC1316
Project area meeting A & B
Location: t.b.a.

PLEASE CHECK THE CRC 1316 WEBSITE FOR UP-TO-DATE INFORMATION ON THE EVENTS.

Twelve years+ SFB-TR 87 come to an end

The SFB-TR 87 started on July 1, 2010. Under its umbrella, the extremely comprehensive topic of *Pulsed High-Power Plasmas for the Synthesis of Nanostructured Functional Layers* has been researched and published extremely successfully over all the years during the following three funding phases until the end of this year.

The German Research Foundation (DFG) supported the joint project as a cooperation between the Ruhr University Bochum (RUB) and the Rheinisch-Westfälische Technische Hochschule Aachen (RWTH) as a collaboration of two scientific locations working at a globally recognized level in their respective fields with a total of more than 36 million euros.

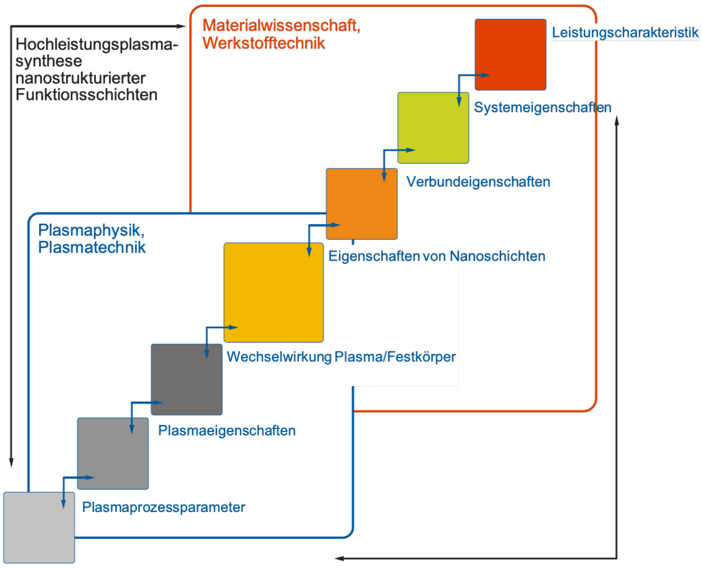
The research topic of the SFB-TR 87 was the plasma synthesis of different material classes, ceramic hard coatings on metal substrates and inorganic quartz-like SiO_2 coatings on plastic substrates. In both cases pulsed plasmas at high power density were used todeposited on the respective substrates at low pressure.

A plastics processing process served as a demonstrator, in which a plastic granulate is further processed into plastic parts at high pressure and at high temperatures in an injection molding process. The molded parts in contact with the plastic melt are subject to high abrasive and oxidative stresses, which were to be equipped with suitable hard coatings based on quaternary CrAlON layers. Furthermore, the task of the SFB-TR 87 was to significantly improve the poor gas barrier properties of the manufactured plastic parts by quartz-like coatings. This resulted in the structure of the SFB-TR 87, which consisted of a "metal route" (project area A), a "plastic route" (project area B) and the plasma route connecting both routes (project area C).

In summary, the two previously separated worlds of plasma research and materials science were to be united by the slogan "from the atom in the gas phase to the synthesized solid with predictable material properties". In this way, the long-standing problem of plasma deposition with previously unknown physical and chemical mechanisms was to be diagnosed and mathematically described. Since the processes are partially based on magnetic field-assisted plasmas, this was an extremely difficult undertaking.

This is all the more true since the field of plasma deposition and synthesis of solids has been worked on and developed in a trail-and-error fashion for decades.

The participating research groups from RUB, as well as Paderborn (UPB) are located in the field of engineering and natural sciences with specializations in the fields of plasma physics and plasma technology, inorganic chemistry, materials science and plasma surface technology.



Legendary "staircase", which started with the plasma process parameters, led to the plasma properties and then to the interaction of the plasma with the solid.

The legendary "staircase", which started with the plasma process parameters, led to the plasma properties and then to the interaction of the plasma with the solid, was groundbreaking for our research. In the middle of the "staircase" were the properties of the deposited nanostructured layers, which then led on to the composite properties, the system properties, and ultimately defined the performance characteristics of the coated components.

In detail, these plasma "stair steps" hide such fundamental and central topics as the identification of the reaction partners in the gas phase, the energy input due to the energetic ions in the solid, the heterogeneous reactions on the solid surface, the energy dissipation in the material but also charge states at the surfaces as well as the magnetization of the electron component. On the material side, on the other hand, the following topics were addressed: first, the phase stability of the deposited layers, furthermore the elasticity and plasticity as well as their residual stresses. Surface energy and chemistry were also investigated, and adhesion to the substrate as well as to the plastic melt were essential parameters. Of course, the permeability of plastics to gases also played a central role.

The high power pulsed plasmas were so-called HPPMS (High Power Pulsed Magnetron Sputter Systems) or HiPIMS plasmas, capacitively coupled multifrequency high frequency (MFCCP) plasmas, inductively coupled high frequency plasmas and pulsed microwave plasmas.

Both the plasmas and the synthesized materials were characterized with partly unique quantitative diagnostics and analytics but also new simulations and models. These had to be partly newly established (gyrokinetics, quantitative OES, laser spectroscopy, large-scale measurement of residual stress, quantum mechanical material design, ...), but partly also made available to the SFB via large procurement requests (atom probe, IR-RAS).

All in all, this cooperation between the plasma groups of the RUB and the materials sciences of the RWTH, supported by the Bochum materials sciences and inorganic chemistry and the technical chemistry from Paderborn, was an extremely fruitful, pioneering collaboration that was completely new at the time. The SFB-TR 87 showed and proved that it makes a lot of sense to tackle hitherto unsolved problems in an interdisciplinary way, to adopt new methods and to overcome supposed barriers across scientific fields.

Thus, the era of the SFB-TR 87 comes to an end, the newly created cooperations, friendships and interests will be the basis for many further research projects.

Peter Awakowicz, spokesperson of the SFB-TR 87

PhD Degree of Vera Bracht & Lars Schücke

Two projects of the CRC 1316 are happy to congratulate their PhD students for their successful degree.

Vera Bracht has written her thesis within project B5 of the CRC 1316 on the “Characterisation of Single Microdischarges during Plasma Electrolytic Oxidation of Aluminium”. After her disputation on 22nd July, there was a champagne reception in the ID courtyard and a small celebration with about 75 people.

In addition, Lars Schücke has completed his dissertation as part of the A7 project, which is a collaboration between Plasma Engineering (AEPT) and Industrial Chemistry (LTC). He defended his thesis with the title “Analysis of Reaction Kinetics in a Surface Dielectric Barrier Discharge for the Conversion of Volatile Organic Compounds” on July 15th. His thesis is part of the overall goal of project A7, where a basic understanding of the used dielectric surface discharge and the addition of complementary catalysts is focused. His main research topic was the determination of the specific mechanisms and reaction pathways of the plasma process which contribute to the production of reactive oxygen and nitrogen species, as well as the subsequent pathways for oxidation of volatile organic compounds.

Lars Schücke, project A7 of the CRC 1316
& PR team of the SFB-TR 87 & CRC 1316

Honours

Prof. Dr. Jochen Schneider wins Rudolf Jaeckel prize 2022

Project leader of A3 and spokesperson of the project area A (also known as the 'A-team') within the SFB-TR 87, Prof. Dr. Jochen Schneider, has won the Rudolf Jaeckel Prize this year. In recognition of his outstanding achievements in the fields of science and technology supervised by the DVG (German vacuum society), in particular for his outstanding scientific contributions and pioneering work in the field of computer-based modeling for PVD layer development.

Prof. Dr. Jochen Schneider (r) with DVG President Prof. Dr. Sven Ulrich, Foto: @EFDS

The award ceremony of the Rudolf Jaeckel Prize 2022 took place during the 18th International Conference on Plasma Surface Engineering PSE in Erfurt.

For the award ceremony at the PSE, Prof. Schneider was able to give an insight into his research work with his award lecture "Quantum mechanically guided coating materials design", certainly also showing the importance of vacuum technology for his scientific success.

Congratulations to this honour!

Dr. Laura Chauvet at Plasma Catalysis Meeting

Dr. Laura Chauvet from Project A3 of CRC 1316 received the poster award for the best poster for her contribution "Mass spectrometric measurements of the plasma catalytic conversion of n-butane at atmospheric pressure". In addition to Dr. Chauvet, three other colleagues from the physics and chemistry departments of CRC1316 participated in the International Symposium on Plasmas for Catalysis and Energy Materials, held in Liverpool, UK, in July 2022.

Dr. Laura Chauvet from project A3 of the CRC 1316

Henrik van Impel's outstanding Bachelor thesis

Congratulations to Henrik van Impel, who won the student award of Ruhr University Bochum with his bachelor thesis "Diagnostics of atomic oxygen in a micro-cavity plasma reactor". He received his certificate during the yearly celebration of the University hosted by the Rector of the University.

In his bachelor thesis, Mr. van Impel used actinometry to investigate the formation of atomic oxygen in a plasma array reactor. With his finding, he made an important contribution to project A6 in CRC 1316.

Henrik van Impel from project A6 of the CRC 1316

Chair of Experimental Physics II receives multiple honours at Faculty celebration

The Physics and Astronomy Department's Faculty Celebration is held annually. Here the graduates of the last year are honored. The ceremony if organized by the different chairs of the department. This year, the chair of Experimental Physics II with the Plasma Interface Physics group had the privilege of hosting the event. The celebration was on October 21st 2022 in the large lecture hall of the Department of Physics. This is a good opportunity to introduce the research field and to present the current research topics.

The event was moderated by Maike Kai and Philipp Maaß. Prof. Dr. Achim von Keudell and Prof. Judith Golda presented their research and some plasma physics experiments.

Maike Kai and Philipp Maaß

As a highlight, Dr. Katharina Laake (born Grosse) from the B7 project of the CRC 1316 gave a very descriptive and target group-oriented lecture (as award lecture for receiving the dissertation prize of the Wilhelm and Else Heraeus Foundation) on the topic "Temporal Evolution of Nanosecond Pulsed Plasmas in Water". The award was presented to her during the event by the Dean of Studies of the Faculty, Prof. Dr. Heiko Krabbe.

Prof. Dr. Judith Golda and Dr. Katharina Laake

Afterwards, the lecturers of the faculty were honored. Here, Prof. Dr. Judith Golda received the lecturer award of the student council. The award is given to the most popular lecturer of the last year among the students.

Finally, PD Dr. Tsanko Tsankov from project A2 of CRC 1316 received his habilitation certificate. He accepted his habilitation entitled "Kinetics of Non-Equilibrium Plasmas" at the faculty on November 21st.

Congratulations to all!

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

Bond formation at PC | X Interfaces

(X = Ti, Al, TiAl) probed by XPS and DFT Molecular Dynamics Simulations

Lena Patterer, Pavel Ondračka, Dimitri Bogdanovski, Leonie Jende, Stephan Prünte, Stanislav Mráz, Soheil Karimi Aghda, Bastian Stelzer, Markus Momma, Jochen M. Schneider

To systematically study the interfacial bond formation between polycarbonate (PC) and different metallic thin films (Ti, Al, TiAl), correlative experimental and theoretical investigations were carried out.

Thin layers of these metals were deposited onto PC substrates by direct current magnetron sputtering and the forming interfaces were subsequently analyzed by X-ray photoelectron spectroscopy (XPS). In addition, density functional theory molecular dynamics (DFT-MD) simulations of a PC dimer interacting with the corresponding metallic surfaces were carried out to compare with the experimentally detected bond formation.

To this end, selected configurations at various simulation times were used to determine changes in the chemical state of the polymer. Consistent with DFT predictions, XPS data indicate a high reactivity of Ti towards PC: Reactions between Ti atoms and all functional groups of PC are observed, resulting in the formation of interfacial C-Ti as well as (C-O)-Ti bonds for Ti and TiAl thin films. In contrast, Al is less reactive since only (C-O)-Al bonds with the carbonate group are formed at the interface. However, integrated crystal orbital Hamilton population (ICOHP) calculations indicate a significantly higher interfacial bond strength for (C-O)-Al bonds compared to the (C-O)-Ti and C-Ti bonds (ICOHP differences up to 2.1 eV). Consequently, the density of interfacial bonds is significantly higher for Ti compared to Al, but (C-O)-Al bonds are stronger. By multiplying the experimentally determined relative interfacial bond concentration with the theoretically determined maximum bond strength as an indicator for adhesion, the PC | Ti interface exhibits a ~ 1.9 times larger value than the PC | Al interface and a ~ 1.4 times larger value than the PC | TiAl interface.

From this data, we predict, that Ti thin films are the best choice for an adhesion layer compared to Al and TiAl layers on PC. These new insights are of fundamental interest to the interaction model of SFB-TR87.

Lena Patterer

About the author

Lena Patterer is part of project A3 of the SFB-TR 87. Her PhD is about the interfacial bond formation of thin films sputtered onto polycarbonate within the group Materials Chemistry of Prof. Jochen Schneider.

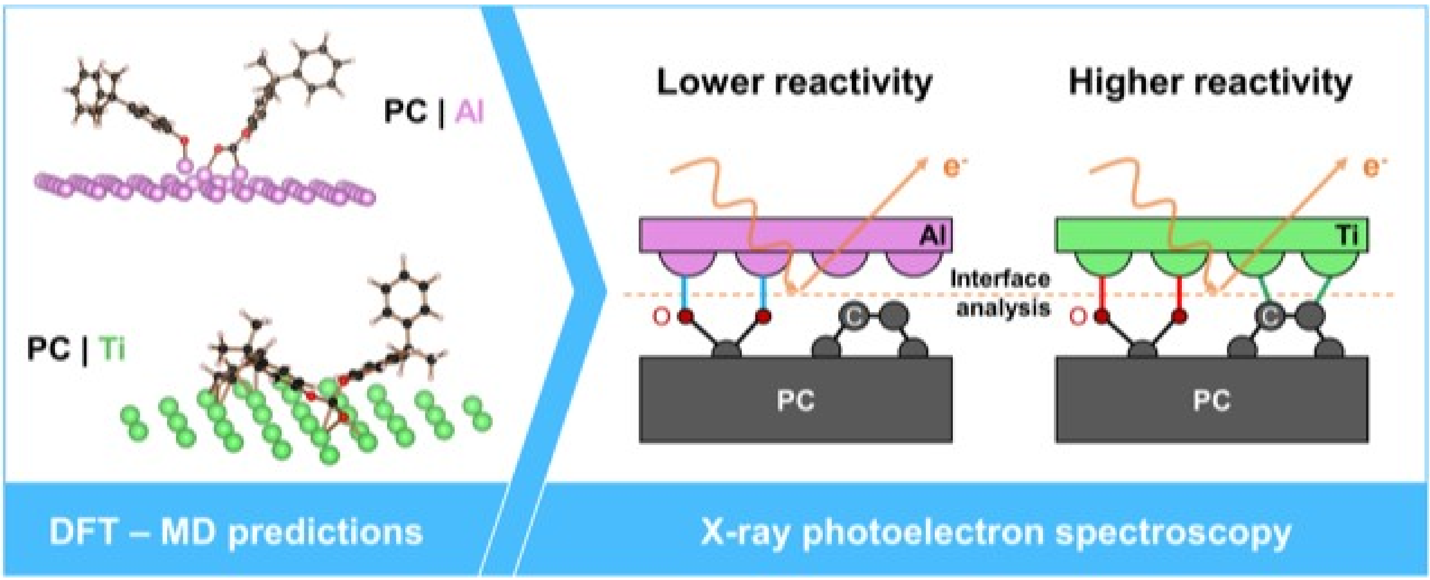


Figure 1: Good agreement is evident for the simulated and experimentally detected bond formation at the PC | Al and PC | Ti interfaces

Research Seminar Report

Materials discoveries at extreme conditions: from curiosity driven research to advanced functionalities

Prof. Igor Abrikosov, head of the Theoretical Physics Division at Linköping University gave a Zoom workshop on the topic of 'Materials discoveries at extreme conditions: from curiosity driven research to advanced functionalities' on 11 August 2022. He presented collaborative materials exploration of oxides and nitrides by theory and experiment at pressures of up to 1 TPa. These materials exhibit fascinating crystallochemistry and physical properties which challenge accepted concepts like Pauling's rules and the concept of valence. For example oxygen was found to have a formal valence less than 2 in high-pressure cubic FeO_2 and complex Fe_3CO_7 carbonate. The reduction of oxygen valence from 2 to 1.5 has been reproduced and explained by density functional theory calculations. Moreover, the group of Prof. Abrikosov discovered several novel nitrides by combining theoretical simulations with experiment, broadly varying composition, temperature and pressure. However, the need to recover the synthesized material at ambient conditions represents the major challenge of such high pressure synthesis in terms of application. The feasibility of the presented approach has been demonstrated for the case of metallic, but incompressible, very hard rhenium nitride pernitride which was discovered at 40 to 90 GPa pressure and a route for scale-up of the synthesis was presented. Finally, the high-pressure synthesis can be used in a search for layered materials which are precursors of novel 2D-materials. For example a monolayer of the triclinic phase of beryllium tetranitride, the beryllonitrene, was suggested as a qualitatively new class of 2D materials that can be built of a metal atom and polymeric nitrogen chains and host anisotropic Dirac fermions. The discussed topics were especially interesting for the mechanical model of SFB-TR 87.

Marcus Hans, project A3 of the SFB-TR 87

New Scientists within the CRC 1316

Florens Grimm studied physics with focus on particle physics at Ruhr University in Bochum. He wrote his master thesis at the chair for experimental physics I (EPI AG), where he performed polarisation measurements on solid targets at a nuclear magnetic resonance setup using a vector network analyzer. Starting June 2022, he made the move to plasma physics by joining project B5 (CRC 1316) as a PhD student, where he will develop a global model for the single microdischarge (SMD) setup with a focus on implementing a two -region model and creating a reaction set which better reflects the chemical processes during plasma electrolysis. The model framework will also be used to perform parameter studies to support the experimental side of the B5 project.
In turn, the measurements done on the SMD setup will be used as input parameters for the simulations.
The final goal of the B5 project is a deeper understanding of plasma electrolysis and its intricacies.

Steijn Vervloedt studied Applied Physics at the Fontys University of Technology and obtained his M.Sc. at the Eindhoven University of Technology (TU/e). For both degrees, he did his graduation project in a plasma based gas conversion related projects. At DIFFER, he studied the NH_3 synthesis in an electrochemical plasma reactor, where ammonia was formed with H_2O and N_2. Later, in the group Plasma and Materials Processing at the TU/e, he studied the influence of O_2 to a CO_2 low pressure glow discharge using infrared absorption spectroscopy.
In the beginning of April 2022, he started as a PhD-student in the A3 project at the Ruhr-University Bochum. Here, he will continue studying the conversion of gases – such as CO_2 – in a plasma reactor, but now the focus will lie on examining surface processes for plasma -catalysis.

Anna Lena Schöne studied electrical engineering with focus on plasma technology at the Ruhr University in Bochum. During her bachelor project and bachelor thesis, she developed the single microdischarge setup for plasma electrolytic oxidation (PEO - project B5 of CRC 1316) and performed optical and electrical measurements. In her master's thesis, she worked on project A7 (CRC 1316) to investigate gas flow effects in surface dielectric barrier discharges with schlieren measurements as well as experiments to inactivate bacteria. In May 2022, she started as a PhD student in project B11. Here, she will develop a model to simulate the plasma and liquid chemistry of the capillary jet for application in plasma-driven biocatalysis. The validation of the model, by comparison with results from Steffen Schüttler (PIP) and Sabrina Klopsch (AMB), will allow the prediction of reactive species concentrations of even non-measurable species and, therefore, a selective and energy-efficient species production.

Lukas Forschner studied chemistry at Ulm University. In 2020, he joined the Plasma group at the Institute of Electrochemistry, where he completed project works and his Master thesis. The thesis concerned the electric field in the electrolyte during high voltage electrolysis and acts as a basis for current and future research.
In March 2022, Lukas started his PhD studies in project B12 which investigates the influence of in-liquid plasma both on the electrolyte and the electrode surface. Within this project, he is mostly interested in the changes in the electrolyte due to the plasma, specifically the electric field, temperature and reactive species like hydrogen peroxide, and how these parameters influence the (re)structuring of the electrode.

Gabriel Boitel-Aullen studied chemistry at Sorbonne University in Paris. He mainly focused on molecular electrochemistry, physical and material chemistry, but he also worked on microbiological systems during his Bachelor thesis and in computational chemistry during his Master thesis. In his PhD, he developed new electrochemical methodologies for understanding fast and complex mechanisms inside supramolecular assemblies.
In October 2022, he joined Kristina Tschulik's research group in the Ruhr University Bochum to work on nanoscale electrochemistry. His main focus is the elaboration of bimetallic nanoparticles in reverse micelles nanoreactors, for electrocatalysis and sensing applications. Since then, he is part of the B13 project of the CRC 1316, whose aim is to produce configuration-controlled nanoparticles by plasma-induced reduction of metallic salts within the nanoreactors.

Siqi Yu studied plasma physics at the Dalian University of Technology. Her Master's thesis was about the investigation of surface charge in surface dielectric barrier discharge. Since September 2022, she starts working as a phD on project A3 which focuses on the excitation transfer between molecules in transient atmospheric pressure plasmas and its impact on plasma chemistry. The focus of her work is the investigation of elementary plasma catalysis mechanisms during the production of nitrogen oxidation.

Simon Homann studied energy and materials physics at TU Clausthal, focusing mainly on materials processing and functionalisation. During the Bachelor's phase, he first came into contact with plasmas to deposit silicon dioxide layers on graphene and steel using PECVD processes. Later throughout his Master's degree, he worked in a start-up company, PlasmaGreen GmbH, which specializes in plasma-assisted VOC removal.
Since November 2021, he has been working on the B4 project, which focuses on atomistic modelling of plasma surface interactions. His main method of choice is molecular dynamics simulations. The project has the goal of investigating the impact of plasma-induced vibrational excitation of molecules on surface processes, especially in the context of catalysis.

Hanna Poggemann studied material physics at the TU Clausthal with specialization in biological physics during her master's degree. After working in the field of experimental protein physics she changed to theoretical chemistry for her PhD at Ulm University. Since April 2022 she is working as PhD student on the plasma biocatalysis project (B8) of the CRC 1316.
Her studies focus on the theoretical investigation of enzyme plasma interactions and the identification of new enzymes for biocatalysis. Furthermore she studies the effect of plasma species on the solvent and the substrate with Molecular Dynamics simulations.

Paolo Cignoni studied chemistry at the University of Milan. He worked on the synthesis and characterization of palladium nanoparticles during his Bachelor thesis. In his Master thesis he focused on the development of novel niobium homogeneous catalysts for dinitrogen photoreduction.
In June 2019, he joined Kristina Tschulik's group at the Ruhr-University Bochum as PhD student working on synthesis and characterization of bimetallic nanoparticles and reaction induced modification of bimetallic electrocatalysts. Since July 2022 he is working on project B13 of the CRC 1316 focusing on the plasma induced nucleation of reverse micelles as a novel pathway for the synthesis of bimetallic nanoparticles.

Propagation of nanosecond plasmas in liquids

Streamer velocities and streamer lengths

Elia Jüngling, Katharina Laake (b. Grosse), Achim von Keudell

Project B7 of the CRC 1316 investigates the reaction chemistry of plasmas in liquids interacting with surfaces. Plasmas in liquids are used for many different applications, including water treatment, plasma medicine and plasma-supported electrolysis. [1]

The discharge is created by applying a short high-voltage pulse to an electrode immersed in distilled and de-ionized water. The voltage pulse with a duration of 10 ns, a rise time of 2 ns and an applied voltage amplitude of -18 kV to -22 kV then causes the formation of luminous, streamer-like structures propagating through the liquid. The ignition process of these discharges is still not fully understood, but several mechanisms have been proposed in the literature. In our recent study, we investigated the temporal propagation of these streamers by ICCD-Imaging and one-dimensional modelling.

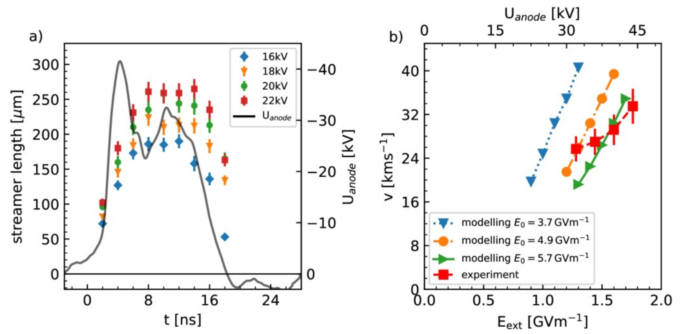


Figure 1: a) Average length of the longest streamer depending on time and voltage (solid points) as well as the correlated voltage waveform (black line). b) Streamer velocities from experiment (red squares) depending on applied voltage and velocities from modelling for different threshold fields.

In the experimental part of this study, the evolution of the longest streamer's length was determined by single-shot images of the discharge at different points in time. One typical example can be seen in Figure 3. Here, every picture for a different moment in time is from a different discharge, due to the limitations of the camera. Therefore, we cannot temporally resolve one streamer, but only look at averaged values over multiple pulses. Figure 1a) shows the temporal development of the average length in the context of the correlated waveform of the applied voltage pulse. The resulting streamer velocities of the initial expansion (from linear interpolation) and also from the modelling for different applied voltages and electric fields respectively can be seen in Figure 1b).

For the one-dimensional modelling of the streamer, we chose a simple drift-diffusion Ansatz. We assumed that the transport is dominated by hydrated electrons and therefore used the transport coefficients of these electrons for our model. The source term is a simple electron impact ionisation term, which is scalable by a threshold value. This is only because ionisation by field effects cannot be implemented in one dimension, but has a similar dominant term, which still allows a comparison to the experiment. The threshold value has, therefore, no direct physical interpretation, but can be seen as a fit parameter. Figure 1b) shows the resulting velocities for different threshold values and Figure 2 the expansion of the negative streamer in the model.

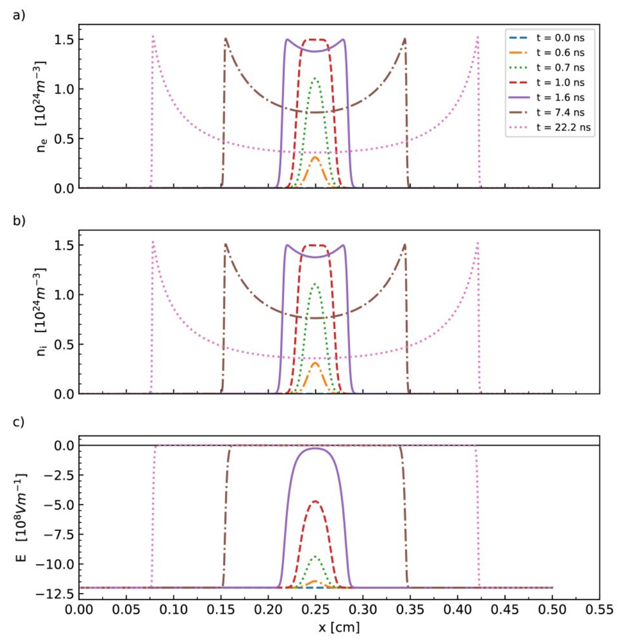


Figure 2: Results of the 1D fluid model for negative streamer propagation in the liquid with transport coefficients of hydrated electrons: a) electron density, b) ion density, c) electric field.

We can summarize our conclusions in two main points:

1) We could reproduce velocities consistent with the experimental data by choosing the threshold field in a way that yields a dominant ionisation source term (shown in Figure 1b)), which is two orders of magnitudes higher than the drift and diffusion terms. Subsequently, the expansion process seems to be dominated by ionisation, which only depends on the absolute value of the electric field. Transport, therefore, would be negligible when assuming it is dominated by hydrated electrons.

2) Figure 1a) shows the linear expansion of the streamers comes to an end, although there is still voltage applied. Further, this maximum extension scales linearly with the applied voltage in the sense, that the applied voltage divided by the maximum extension is constant. This indicates the existence of a necessary condition for the propagation that also scales inverse with the distance to the electrode. We discussed multiple possible quantities, particularly the pressure field, the electrostrictive pressure and the external electric field. We found that out of these, only the electric field can explain this maximum extension well. When the background electric field falls beneath a critical value, propagation is no longer possible. This so-called stability field is well known to determine the maximum streamer length for streamers in gases [2-4]. Here the stability field would be in the order of 10^7 V/m.

In a nutshell, we proposed a dominating local ionisation mechanism at the front of the streamer and the stability field limiting the expansion in space. This work can serve as a basis for further investigation, using more sophisticated models and more detailed experiments on a smaller length scale, in the future.

Elia Jüngling

[1] J. Phys. D: Appl. Phys. **43**, 012003 (2010), doi: 10.1088/0022-3727/43/1/012003

[2] Sov. Phys. JETP 67, 1049 (1988)

[3] Plasma Sources Sci. Technol. **29**, 103001 (2020), doi: 10.1088/1361-6595/abaa05

[4] Arxiv, doi: 10.48550/arXiv.2107.06781

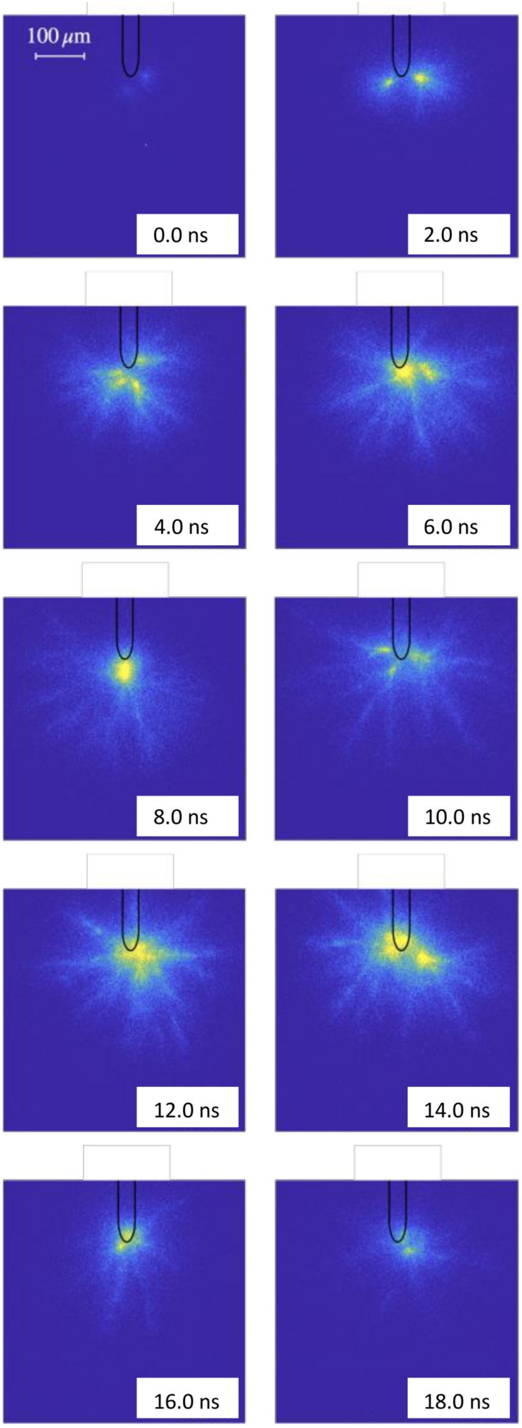


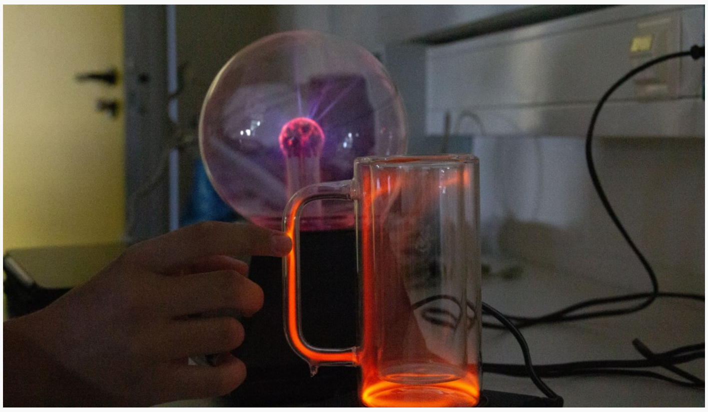
Figure 3: ICCD images of the plasma expansion at different moments in time for a HV output voltage of 20 kV at 2 ns exposure time scaled to absolute brightest emission . The tungsten tip is marked with a black line.

About the Author

Elia Jüngling has completed his Bachelor thesis on the „Propagation of streamers in nanosecond plasmas in water“ in project B7 of the CRC 1316.

New concept introduced in the plasma workshop of the project week

The project week for students at Ruhr University Bochum in grade 8 and 9 is a educational offer of the CRC 1316, Faculty of Physics and Astronomy from RUB and is greatly supported by zdi . From 4th to 7th October, the project week took place with four workshops hosting over 60 high school students.



The concept of the plasma workshop "From plasma to gold coating" was adapted accordingly to feedback by students and workshop leaders from the last years. The focus of the topics was shifted from theoretical work towards application based discussions with exercises to practice and apply newly gained knowledge. The focus has been set to enable the students to plan and execute their research as well as analyse the data and present their findings creatively and self-determined. The workshop leaders and material should guide through the workshop, offering the students a democratic say in the concrete design of the week.

To adapt the material to modern standards and the vast digital resources available for student online, the project guide now includes online resources that can be used for better understanding or diving deeper into different topics by using the QR-codes to access articles and videos. In the future, this guide can also be used with and on tablets and as a digital version, enhancing the interactivity and individualisation of the learning process of the students even further.

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

Large CRC1316 participation in the International Plasma School

The 25th edition of the International Plasma School on Low-Temperature Plasmas took place from 1th to 5th October at the Physics Centre in Bad Honnef. Afterwards, the two-day Master Class on electric propulsion has been held. 76 participants from sixteen nations joined this yearly event. The international chair of the Plasma School was in the hands of Prof. Dr. Holger Kersten and Prof. Dr. Jan Benedikt from CAU Kiel.

The CRC 1316 participations at the plasma school

The extensive program offered various topics to the students: from theory to applied plasma technologies. The lectures (23 from eight nations) were accompanied by a social program that allowed for intensive discussion with the teachers. Every evening there was a question and answer session with the teachers of the day, where an exciting exchange had been held. Hands-on workshops also provided practical experience in the field of spectroscopy.

Moreover, a large number of PhD students from the CRC 1316 and accompanying projects were part of the event this year.

Marina Prenzel, member of the organizing committee of the plasma school

CRC 1316 at the International Conference on Plasma Medicine

In the summer, Dr. Sebastian Burhenn and Steffen Schüttler, together with Sabrina Klopsch and Tim Dirks from the RUB Applied Microbiology group, visited the 9th International Conference on Plasma Medicine (ICPM9) in Utrecht, the Netherlands. Around 250 participants discussed the current state of plasmas in medicine. Topics ranged from "Plasma Agricultural Applications" to "Plasma-Liquid Interactions" to "Plasma-Based Decontamination and sterilisation" and much more.

Steffen Schüttler, Tim Dirks, Dr. Sebastian Burhenn, Sabrina Klopsch (from left to right)

Sebastian Burhenn gave a presentation in the section "Fundamentals of Atmospheric Plasma" on the "Influence of Humidity on OH Distribution in the COST Jet measured by Laser-Induced Fluorescence". Steffen Schüttler contributed to the section "Plasma-Liquid Interactions" with his talk on "Hydrogen peroxide production in water treated with a capillary plasma jet". Sabrina Klopsch and Tim Dirks presented a poster about their work in the field of plasma-driven biocatalysis.

Steffen Schüttler, project B11 of the CRC 1316

Gordon Research Conference with Contributions from Bochum

From July 23rd to July 29th the Gordon Research Conference and Seminar on Plasma Processing and Science (GRC) was held in Andover, New Hampshire. The conference focused on plasmas and their interactions with matter while the seminar focused on investigating multiphase and multiscale plasma-material interactions.

Prof. Dr. Judith Golda, Simon Kreuznacht, Rahel Buschhaus at the GRC (from left to right)

Prof. Dr. Judith Golda from CRC 1316 gave a talk on "State enhanced actinometry in atmospheric pressure discharges". She also organized the Gordon Research Seminar together with Marien Simeni. Moreover, Judith Golda organized the so-called "Power Hour" at the GRC - an event to raise awareness about discrimination against underrepresented groups in plasma physics.

Rahel Buschhaus from project C7 of the SFB-TR 87 presented her paper on "Ion induced secondary electron emission from metal surfaces analyzed in beam experiments" during the research seminar. She had one of the top two presentations in the research seminar and was honored to give her talk again at the research conference to a large audience. In addition, Judith Golda, Simon Kreuznacht, and Rahel Buschhaus gave poster presentations.

Simon Kreuznacht, project Me2H2

On the synergistic use of numerical and analytical work

Earlier this year, the A8 project of the CRC 1316 communicated its work in two publications. Project A8 uses special analytical and numerical methods to define optimized models for jet-shaped plasma sources (such as the COST-Jet). The focus is on both the physical reliability and the numerical efficiency of the models. (The improved performance frees up computational resources that can be used, for example, to describe the complex plasma chemistry in more detail.) The spirit of project A8 is reflected in these recent publications.

The papers named “Simulation and modeling of radio-frequency atmospheric pressure plasmas in the non-neutral regime“ [1] and “Validation of the smooth step model by particle-in-cell/Monte Carlo collisions simulations“ [2] stress the powerful synergy that arises from the combination of analytical models and numerical simulations. Both papers utilize a variant of the kinetic particle-based particle-in-cell/Monte Carlo collisions (PIC/MCC) algorithm and combine the method with separate analytical models. The work on the non-neutral regime applies a hybrid scheme that describes electrons kinetically and solves fluid equations for each ion species. The conclusions drawn from the simulations are confirmed and concretized by mathematical modeling of the non-neutral regime. The paper on the smooth step model is based on the name-giving smooth step model (SSM), an analytical boundary sheath model for capacitively coupled plasmas. The work then utilizes the classical fully kinetic MCC approach for all charged particles to test the fidelity of the smooth step model.

The paper on non-neutral discharges pays attention to discharge phenomena that were ignored up to this work. Capacitively coupled, single-frequency-driven plasmas at atmospheric pressures tend to fail to establish a quasi-neutral bulk region (see fig. 1 a)). The work published by project A8 characterizes such a discharge as a distinguished operation mode. Moreover, a first version of a semi-analytical model for a non-neutral discharge is introduced, and the performance is discussed (c.f., fig. 1). The main result of the work on the smooth step model is presented in figure 2. The SSM perfectly matches the results of the more sophisticated PIC/MCC

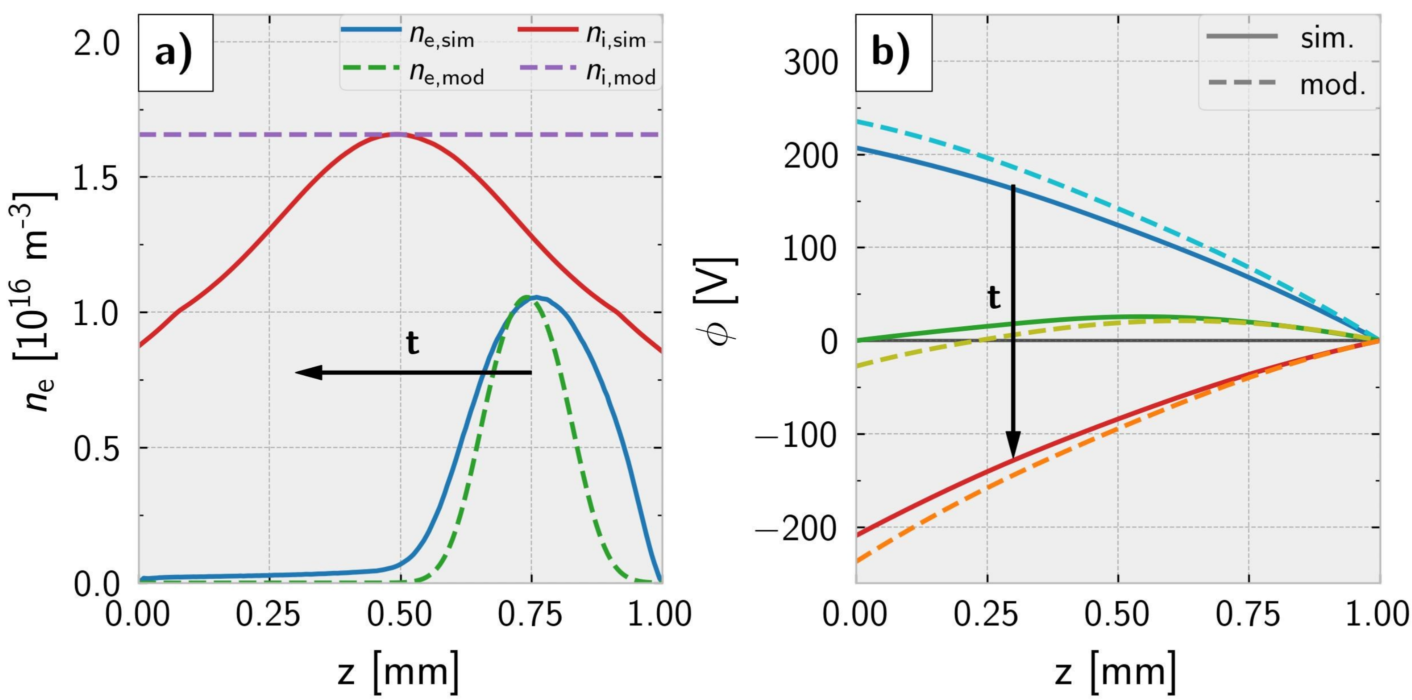


Figure 1: A comparison between the results of a hybrid PIC/MCC simulation, and an analytical model for the non-neutral discharge regime.

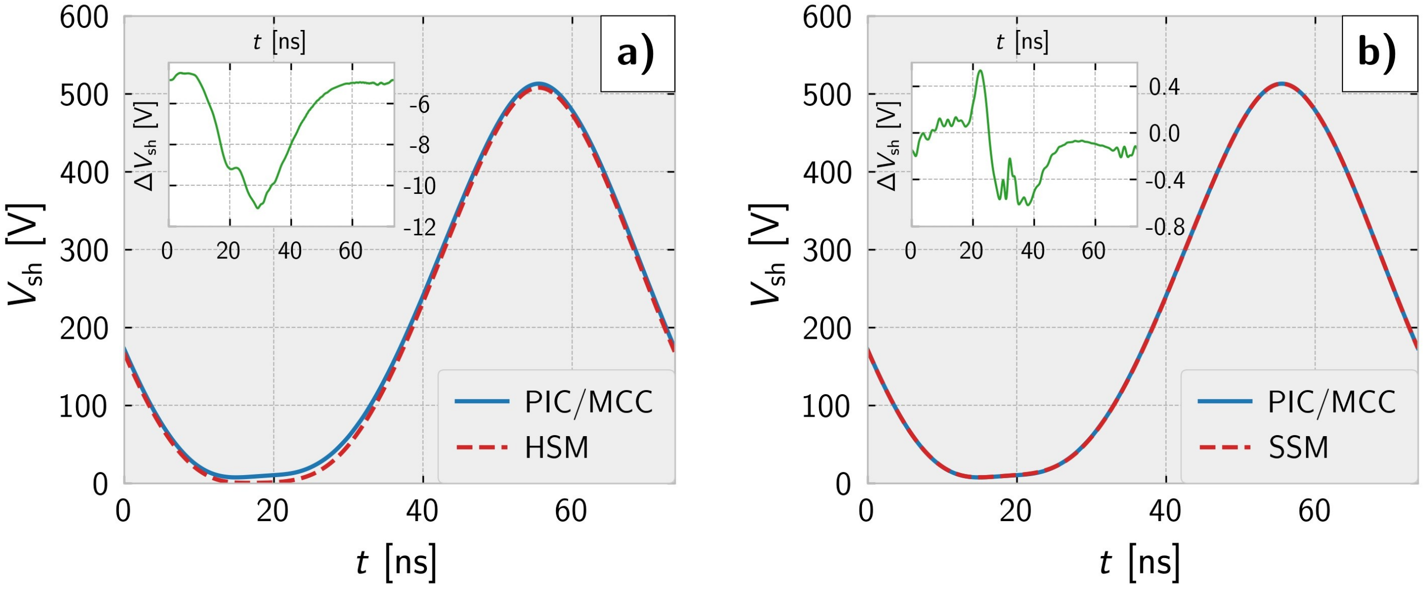


Figure 2: A comparison of the sheath voltage between a PIC/MCC simulation, the hard step model (HSM - a basic boundary sheath model), and the SSM. Copied from [2].

simulation (cf. fig. 2 b)). However, it must be stressed that the SSM is more mathematically complex than other boundary sheath models. As figure 2 a) shows, this subtlety is necessary (i.e., simpler models perform worse). Compared to the results we discussed in figure 1, where a higher disparity between the models is accepted, it sounds contradictory that minor discrepancies now matter. However, it turns out that solely the SSM can describe plasma heating reliably.

In terms of authorship, the CRC 1316 enriched and boosted both papers. The validation of the smooth step model is a cooperation between the staff of A8 and project A4. The work on non-neutral plasmas profited from the ideas of Mercator fellow Zoltán Donkó.

Overall, both papers demonstrate that a detailed analysis based on numerical simulations leads to understanding the respective plasmas. This knowledge is then used to create models that describe the discharges at lower computational costs.

These freed resources allow the realization of more complete models of the respective plasma sources required to investigate complex problems such as plasma catalysis.

[1] Plasma Sources Sci. Technol. 31, 045003 (2022), doi: 10.1088/1361-6595/ac5cd3

[2] Plasma Sources Sci. Technol. 31, 045014 (2022), doi: 10.1088/1361-6595/ac5dd3

Maximilian Klich

About the Author

Maximilian Klich works in project A8 of the CRC 1316. He is doing his PhD on *Modeling and simulation of atmospheric pressure plasmas* within the group Theoretical Electrical Engineering of Prof. Palf Peter Brinkmann.

Workshops from the working group IANiS

Future ideas and directions

Since the SFB-TR 87 is going to terminate by end of 2022, all project area members as well as Mercator fellows were invited to contribute ideas and directions towards future joint research projects in plasma and materials science. Inspired by the established insights of the past and current funding phases, all participants were asked to bring up the most exciting and innovative scientific topics in a two-part workshop 'Future ideas and directions'. The first part took place virtually via Zoom on 13 January 2022 and was focused on short pitches to foster new ideas in a joint brainstorming.

Among the discussed topics were:

- Prediction of cracking in hard coatings utilizing anisotropic damage models and data-driven approaches
- Gas-solid interactions in porous thin films (e.g. SiO_2) studied by near-ambient pressure XPS
- Role of quantum mechanics in understanding plasma-surface interactions
- Kinetic simulations of various technological plasmas
- Tailoring of HiPIMS thin films for antifouling properties in aqueous environments
- In-situ 2-D thin film stress measurements in realtime
- Simulation and data-driven modeling of plasma-surface interactions
- HiPIMS: Is working gas recycling real?

While the participants reviewed challenges presently encountered, in the first part of the workshop the spotlight was on envisioning possible pathways to tackle these. Subsequently, the proposed topics were discussed with respect to overlaps in research questions and a common agenda for potential future proposals in the second part of the workshop on 22 June 2022.

Of special interest were the talks by the Mercator fellows Prof. Christian Mitterer ('How sustainability will drive process, materials and product innovations in surface engineering') and Prof. Ludvik Martinu ('Stress in films and coatings - its understanding and control') as well as Prof. Guido Grundmeier ('HPPMS films for applications in energy conversion'). It should be also mentioned that the second part of the workshop was in particular inspired by interactions of the participants during the intermediate Summit Meeting of SFB-TR 87 in Grainau. Based on these fruitful discussions, new exciting research directions can be expected.

Machine learning in plasma and materials science

Artificial intelligence and big data attracted enhanced interest within the past years not only in the general public, but also in plasma and materials science. A workshop to bring together corresponding activities within SFB-TR 87 entitled 'Machine learning in plasma and materials science' took place virtually via Zoom on 16 September 2022. This workshop was focused on machine learning-based approaches to support experiments, simulations, and predict synthesis-composition-properties relationships. For example, artificial neuronal networks like variational autoencoders have already been used in the present CRC. In this workshop, different applications of machine learning approaches were illustrated by four highlight talks.

Lars Banko (project C2) discussed 'Data-driven high-throughput experimentation using combinatorial material science methods and machine learning' and showed for example how artificial intelligence can aid the identification of phases within X-ray diffractograms. Insights on big datasets with millions of atoms were shown in the talk 'Analysis of atom probe tomography data by 3D computer vision' from Janis Sälker. Especially the automated recognition of patterns, indicating e.g. the onset of thermal decomposition in nitrides, paves the way toward operator-independent data analysis.

Tobias Gergs (project C8) presented 'A plasma-surface interaction surrogate model for the sputter deposition of AlN' and discussed that machine learning enables high physical fidelity predictions of thin film processing on the global process timescale.

Finally, Ali Harandi (project A6) talked about a 'Physics-informed neural network for predicting mechanical behavior of heterogeneous boundary value problems' with a focus on the performance of machine learning approaches compared to conventional finite element modeling.

The workshop was concluded with a round table discussion and the participants agreed to meet again as a working group even beyond the SFB-TR 87.

Marcus Hans and Jan Trieschmann

About the authors

Marcus Hans (left) works in project A3 of the SFB-TR 87. He is group leader Atom Probe Tomography at the Chair of Materials Chemistry at RWTH Aachen.

Jan Trieschmann (right) is Junior Professor for Theoretical Electrical Engineering at CAU Kiel and is PI in project C8 of the SFB-TR 87. He works on physical simulation and data-driven modeling of plasmas andtheir surface interactions.

Jan and Marcus have taken care of the IANiS working group for more than four years.

State enhanced actinometry in the COST microplasma jet

Reactive species such as atomic oxygen play a key role in plasma catalysis, as they can interact with a gas to be treated as well as with a catalytic surface. For this reason, diagnostics are needed to monitor atomic oxygen densities. Typically, this can be done with laser spectroscopic methods such as *two photon absorption laser induced fluorescence* (TALIF). However, optical access for both laser and fluorescence signals is required, which may not always be the case for micro discharges.

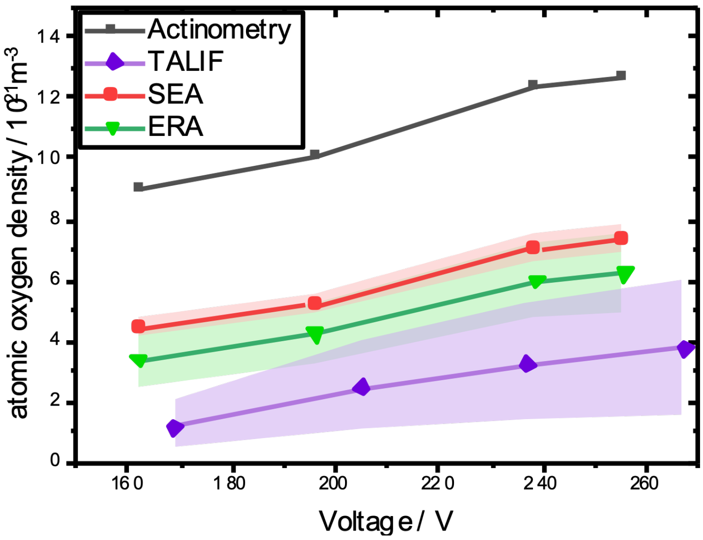


Figure 1: Atomic oxygen density determined by various methods as a function of applied voltage. Colored areas: confidence intervals.
Conditions: 1 slm He, 5 sccm O_2, 0.5 sccm Ar.

Optical emission spectroscopy, specifically actinometry, offers an alternative: Here, the intensity ratio of two spectral lines is used to calculate the atomic oxygen density. However, the calculation is based on a number of assumptions, for example that the excitation from the ground state occurs exclusively by electron impact excitation. This may not be correct especially in the case of oxygen, since dissociative excitation can also be present here.

A solution to this problem was presented by Greb et al: *Energy Resolved Actinometry* (ERA). Here, instead of measuring the emission of two spectral lines, the excitation into three different states is measured. With the help of the Boltzmann solver BOLSIG+, the dissociative part of the excitation can be taken into account and a mean electron energy can be determined.

In a cooperation between the CRC1316 subprojects A6, B2 and B11 we have developed a further progression of ERA: *Helium state enhanced actinometry* (SEA). Here, the measurement is by measuring a helium line at 706 nm instead of the typically used oxygen line at 777 nm. This has a number of advantages: First, the energy measurement can be improved because different parts of the EEDF can be probed due to the highly excited helium state. Second, the state measured at 777 nm is known to be populated by metastable atoms or molecules. To minimize this influence, usually time-resolved measurements must be performed. In the case of SEA, this influence is generally smaller, allowing time-integrated measurements.

To qualify the method, a benchmark against TALIF measurements was performed on the COST-Jet. The absolute densities and relative profiles as a function of the voltage are in good agreement (see fig. 1). Furthermore, mean electron energies known from the literature could be reproduced.

In summary, SEA offers the possibility to measure atomic oxygen densities and mean electron energies also in plasmas where laser spectroscopic methods as TALIF are challenging. In contrast to ERA, SEA offers the possibility of time-integrated measurements and reduces sources of error like excitation by metastables. This makes the diagnostics feasible for a large number of applications in industry and research.

[1] David Steuer *et al* 2022 *Plasma Sources Sciences Technol.* **31** 10LT01

[2] Tristan Winzer *et al* 2022 *Journal of Applied Physics* **132** 183301

David Steuer

About the Author

David Steuer works in project A6 of the CRC 1316. He is doing his PhD on Two-Dimensional Oxygen Distributions in Microplasmas by Optical Methods within the group Plasma Interface Science of Prof. Judith Golda.

GEC— Gaseous Electronics Conference

Conference report

After two years of social distancing and online meetings, 2022 will be known as the year that gave rebirth to on-site conferences. Since the beginning of the year, many conferences have returned, and so has the GEC (gaseous electronics conference). From October 3rd to 7th, the international low-temperature plasma community met in Sendai, Japan.

Almost six hundred papers were presented to five-hundred-fifty participants; the third most papers within the last ten years, and an attendance comparable to the much cheaper online events. Another notable statistic of the conference is the high count of students. Half of

the participants were students, which included Ph.D. students as well as undergrads. With thirty-three contributions, a large group from Bochum and the CRCs attended GEC. Similar to the conference, this group had a dominant share of Ph.D. and undergrad students.

At least four parallel sessions were conducted to fit the numerous contributions into the five days available. Scientific highlights of the conference were the workshops conducted on Monday and the price talks.

Andrew Gibson, Lars Schücke and Jan Trieschmann (former two CRC 1316, latter SFB-TR 87) were invited to present their research. Julian Schulze (PI in both SFBs) chaired and organized the GEC, and five people from the consortia were chosen as session chairs. All in all, the large share of people and their valuable contributions caused the CRCs to impact the conference meaningfully.

Eventually, something apparent to everyone who has visited Japan has to be mentioned. Japan has a rich culture, offers delicious food, and beautiful nature. This diversity made all free-time and non-science-related activities in the evenings a delight. The wholesome and successful experience is reflected in the happy faces in the picture left hand side.

Maximilian Klich, project A8 of the CRC 1316

GEC in Japan was a success for CRC 1316 students

Bachelor's student Arisa Bodnar from the Ruhr University won the Student Poster Award at this year's APS Gaseous Electronics Conference in Sendai, Japan, with her contribution "Improving the decomposition of polluted air streams using additional metal plates in a dielectric double-surface discharge system with multiple

Tobias Gergs

Arisa Bodnar

electrodes." In this poster contribution, Arisa investigates surface dielectric barrier discharges (sDBD) that are used to decompose volatile organic compounds (VOCs) from industrial exhaust gases (e.g., chemical plants).

Furthermore, PhD student Tobias Gergs from the Ruhr University Bochum won the GEC Student Award for Excellence at the GEC in Sendai, Japan, with his contribution "Dynamic surface surrogate model trained on atomistic data of AlN sputter depositions".

Sebastian Wilczek, project A5 of the CRC 1316

Exchange with Institute of Plasma Physics of the Czech Academy

From October 17th—19th, Pia Pottkämper and Dr. Katharina Laake from project B7 (CRC 1316) visited the Institute of Plasma Physics of the Czech Academy (IPP) of Sciences as part of an exchange visit. Motivation for this exchange was the similar research topic of both groups. Previously from October 12th—13th Dr. Petr Bílek from that same Institute had visited the EP2 chair to give a talk on the recent results of his groups investigations of nanosecond pulsed plasmas in water. At the IPP they were invited to visit the labs and experiments. They had the chance to discuss and compare their research of nanosecond pulsed plasmas in liquids. According to that topic, Katharina Laake gave a talk regarding the “Temporal evolution of nanosecond pulsed plasmas in water” at the Institute. During their stay they also had the chance to explore the city of Prague with their hosts.

Pia-Victoria Pottkämper, project B7 of the CRC 1316

Pia-Victoria Pottkämper & Dr. Katharina Laake from project B7 of the CRC 1316 at IPP in Prague

New cooperation between project B7 and the Forschungszentrum Jülich

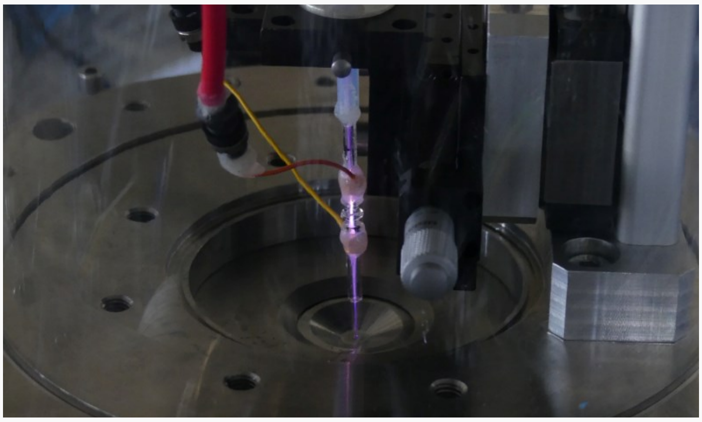
Pulsed plasmas in liquids are intensively investigated in project B7 of the CRC 1316. One possible application of these plasmas is the generation of nanoparticles directly in the liquid. These particles are deposited from the electrode material during the plasma ignition and thus particles of different sizes are generated. Now coopera-

tion with the Forschungszentrum Jülich, a method is to be developed to to produce composite nanoparticles during plasma operation in liquids. in liquids during plasma operation. For this purpose, the researchers Dr. Katharina Laake and Elia Jüngling from project B7 have travelled to Forschungszentrum Jülich to produce the first prototypes for electrode tips, which will which can later be used to produce composite nanoparticles.

Katharina Laake, project B7 of the CRC 1316

Continuous exchange between Bochum and GREMI laboratory

The DAAD exchange program (part of a PROCOPE project) between Prof. Judith Golda from Ruhr University Bochum and Prof. Claire Douat from GREMI allowed several exchange visits between both groups. The exchange focuses on the study of the role of CO in the treatment of biological substrates.



The photo shows the plasma source directly above the mass spec orifice in a controlled gaseous atmosphere.

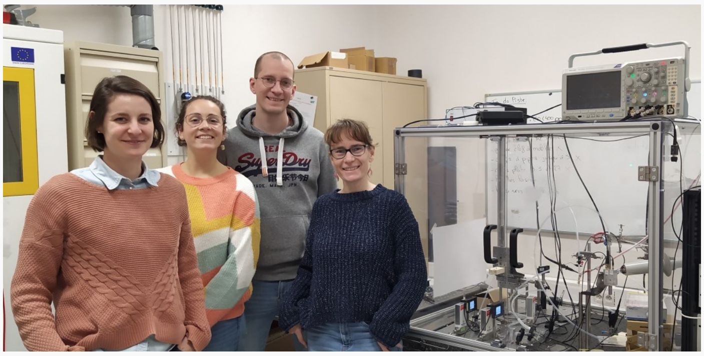
Cold atmospheric pressure plasmas could provide a well-controlled local source of small-dose CO that can be directly guided to the treatment zone. The aim of the project is to investigate the production pathways and the role of the CO molecule during the plasma treatment of biological material. Possible synergism of CO and plasma produced species such as electric fields, ions and electrons, photons and other neutral radicals are analysed.

In detail, several exchange visits from both labs were realized. In July, Jun.-Prof. Judith Golda, Dr. Laura Chauvet and Daniel Henze from the CRC 1316 were guests in the laboratory of Prof. Claire Douat at the GREMI in Orléans. In a joint measurement campaign, two different atmospheric pressure plasma jets were being tested. They measured the production of CO at different operating conditions with a gas analyser.

Dr. Laura Chauvet (RUB), Daniel Henze (RUB), Prof. Dr. Claire Douat (GREMI), Prof. Dr. Judith Golda (RUB), Eloïse Mestre (GREMI) in GREMI in July; from left to right

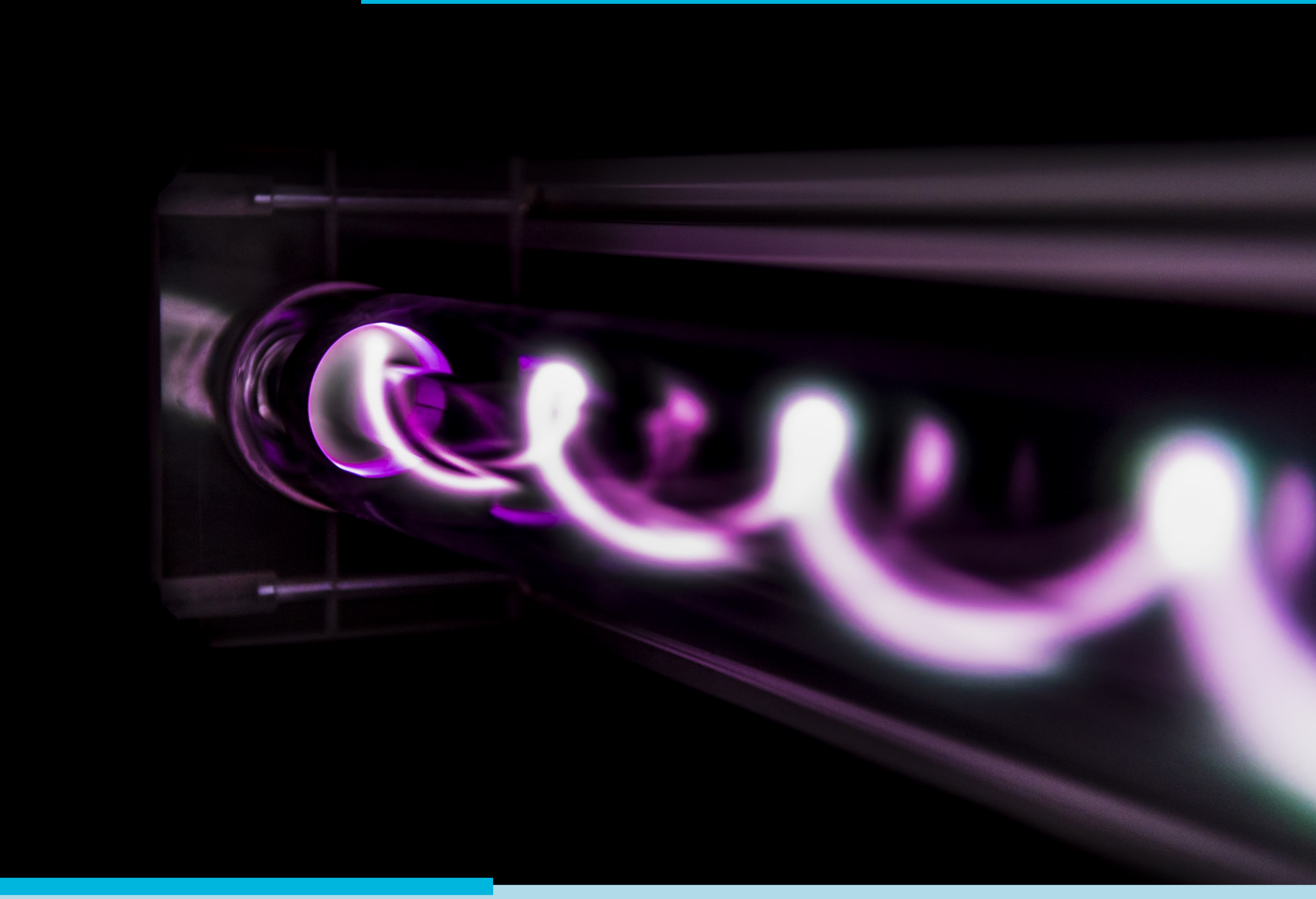
In October, directly after the Plasma School in Bad Honneff, Eloise Mestre visited the PIP group. The second measurement campaign focused on the measurement of plasma produced CO in a kHz jet source using mass spectrometry.

Finally, Jun.-Prof. Judith Golda and Dr. Sebastian Burhenn stayed in the laboratory of Prof. Claire Douat at the GREMI in Orléans for a joint research campaign in November again. This time, the work was focused on the measurement of plasma-produced carbon monoxide affecting human hemoglobin.



Prof. Dr. Judith Golda (RUB), Eloïse Mestre (GREMI), Dr. Sebastian Burhenn (RUB), Prof. Dr. Claire Couat (GREMI) in November in GREMI; from left to right

Judith Golda, project A6, B2 and B11 of the CRC 1316



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