

# NEWSLETTER

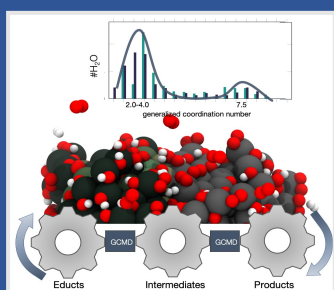
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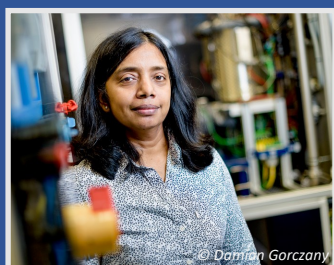
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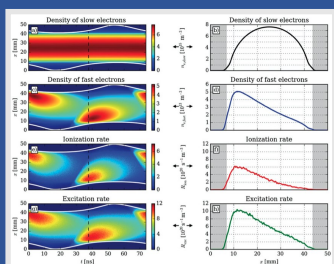
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9<sup>th</sup> newsletter in times of Covid-19

Although we are all currently facing many new challenges, some progress in research has been made in the recent months. Many have used the time at home to work on papers, to push forward with final theses, and to delve deeper into the subject matter. So, the last few weeks have not only presented challenges, but also opportunities to the most of us.

This also includes the development of digital structures in the research collaborations. Since meetings could no longer be held on site, the agendas and presentations were changed. Hence, the exchange, which is highly appreciated by many, could continue in the form of an online meeting. With the gradual opening of the laboratories, experiments can now be resumed. These were certainly rarely put back into operation with so much joy and motivation.

In this newsletter, we have chosen the topic of internationalisation. Even though this was chosen before the Covid-19 situation, this time has once again underlined

the importance of international cooperation and exchange. This does not only enable more effective research, but also strengthen the research community by interlinking the expertise of individual researchers.

Internationalisation also means cultural challenges and different habits. Here, it is important to break down barriers and get to know other countries in order to establish a barrier-free exchange in the long-term. Research stays abroad are a great opportunity to do this, but also to get to know the similarities and differences of research in detail through field reports. Therefore, this newsletter will not only present research progress but also reports on experiences.

Stay healthy and take advantage of the opportunities that are opening up for us during this time!

*Maike Kai, public relations  
for the SFB-TR 87 and CRC1316*

*Research seminar at MCh RWTH*

## Microstructure characterization of transition metal-based nitride coatings

**Dr. Christina Wüstefeld** from TU Bergakademie Freiberg gave a seminar on *Microstructure characterization of transition metal-based nitride coatings* on December 2<sup>nd</sup>, 2019.

After introducing the basics of glancing incidence X-ray diffraction, Dr. Wüstefeld presented her work about the influence of Al content and of applied bias voltage on the microstructure of cathodic arc-evaporated  $Ti_{1-x}Al_xN$  coatings. Chemical compositions of  $x = 0.4, 0.5, 0.6$  and  $0.67$  and substrate bias voltages of  $-20, -40, -80$  and  $-120$  V were utilized and the coatings were characterized regarding phase composition and mechanical properties.

High bias voltages were found to suppress the formation of the softer wurtzite (w-)AlN phase due to the stress-induced stabilization of cubic AlN. In contrast, a high Al content enhances w-AlN formation, which can also improve the mechanical properties by reducing the size of the nanocrystals significantly. These findings were interesting and insightful for the mechanical model within the SFB-TR 87.

*Lena Patterer, project A3 of the SFB-TR 87*

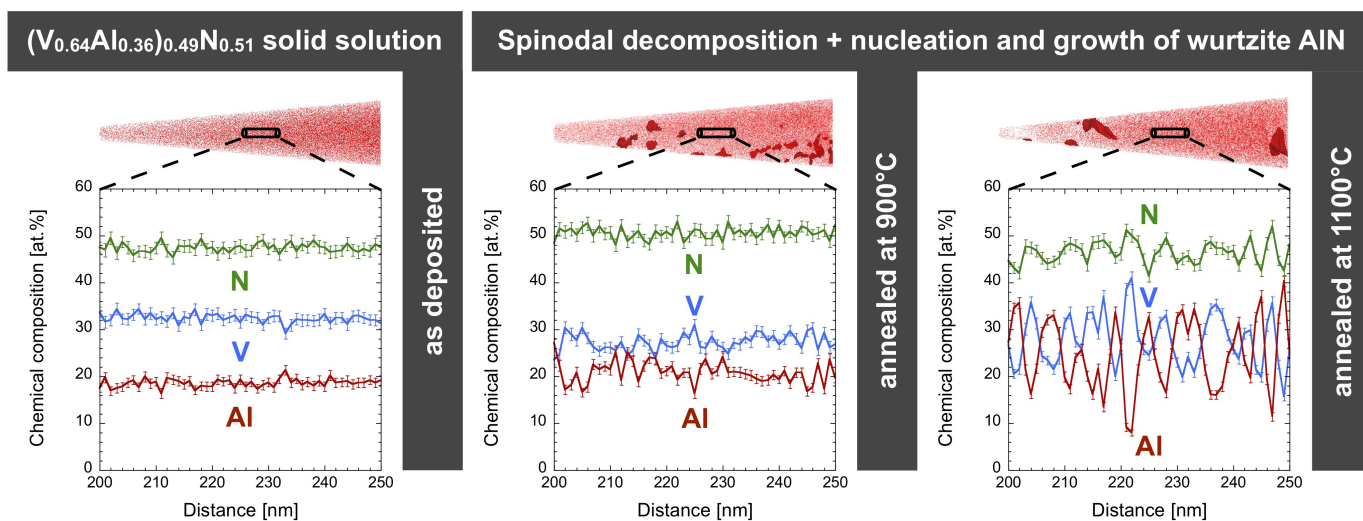
## Do metastable (V,Al)N thin films decompose spinodally upon annealing?

While the spinodal decomposition of (Ti,Al)N is well known for almost 20 years and utilized to induce age hardening of protective coatings under operation at elevated temperatures, the occurrence of spinodal decomposition in (V,Al)N has been under debate. Recently, the question whether (V,Al)N thin films decompose spinodally upon annealing has been answered in a publication from project A3 of the SFB-TR 87 *Spinodal decomposition of reactively sputtered  $(V_{0.64}Al_{0.36})_{0.49}N_{0.51}$  thin films*<sup>[1]</sup>.

The decomposition mechanisms of metastable cubic (c-)  $(V_{0.64}Al_{0.36})_{0.49}N_{0.51}$  thin films, grown by reactive HPPMS,

at 900°C. These chemical modulations are quantified by atom probe tomography and maximum variations of  $x$  in  $V_{1-x}Al_xN$  are in the range of 0.36 to 0.50 (see Figure 1).

The magnitude of the compositional modulations is enhanced after annealing at 1100°C as  $x$  varies on average between 0.30 and 0.61, while the modulation wavelength remains unchanged at approximately 8 nm. Based on DFT data, the local  $x$  variation from 0.30 to 0.61 would cause lattice parameter variations from 4.111 to 4.099 Å. This difference corresponds to a shift of the (200) peak from 44.0 to 44.1°. As the maximum



**Figure 1:** Evidence for spinodal decomposition of  $(V_{0.64}Al_{0.36})_{0.49}N_{0.51}$  based on atom probe tomography.

have been investigated by combination of structural and compositional characterization at the nanometer scale with DFT calculations. Based on thermodynamic considerations of  $\partial^2\Delta G/\partial x^2 < 0$ , spinodal decomposition is expected for c- $V_{1-x}Al_xN$  with  $x \geq 0.35$ . While no indications for spinodal decomposition are observable from laboratory and synchrotron diffraction data after annealing in Ar atmosphere at 1300°C, the formation of wurtzite (w-)AlN is evident after annealing at 900°C by utilizing high energy synchrotron X-ray diffraction. However, the complementary nature of elemental V and Al maps, obtained by energy dispersive X-ray spectroscopy in scanning transmission electron microscopy mode, imply spinodal decomposition of c- $(V_{0.64}Al_{0.36})_{0.49}N_{0.51}$  into V- and Al-rich cubic nitride phases after annealing

decomposition-induced peak separation magnitude of 0.1° is significantly smaller than the measured full width at half maximum of 0.4°, spinodal decomposition cannot be unraveled by diffraction data. However, consistent with DFT predictions, spinodal decomposition in c- $(V_{0.64}Al_{0.36})_{0.49}N_{0.51}$  is revealed by chemical composition characterization at the nanometer scale.

Marcus Hans, project A3 of the SFB-TR 87

- [1] M. Hans, H. Rueß, Z. Czigány, J. Krause, P. Ondračka, D. Music, S. Evertz, D. M. Holzapfel, D. Primetzhofer, J. M. Schneider, Surf. Coat. Technol. 389 (2020) 125641, <https://doi.org/10.1016/j.surfcoat.2020.125641>

## Two PhD students profit from research stay at Hamaguchi Lab, Center for Atomic and Molecular Technologies, Osaka University, Osaka



From October to December 2019, I was able to join the lab of Prof. Satoshi Hamaguchi at the Center for Atomic and Molecular Technologies in Osaka, Japan.

My field of research is applied microbiology and my focus is on biocatalytic reactions with non-thermal plasmas.

Using numerical simulations, I studied the propagation of plasma-induced reactive species in liquids to gain an insight on the depth of penetration and concentration of these species. This knowledge will help to understand the interaction between plasmas and enzymes that are studied in project B8 of the CRC 1316, specifically to protect the enzymes from inactivation and to drive biocatalysis.

The research stay in Japan was very helpful to deepen my knowledge for my main research question.

*Abdulkadir Yayci, project B8 of the CRC 1316*

I have visited Hamaguchi Laboratories at Osaka University in Japan for 3 months. The lab exchange was funded partially by the CRC-1316 and the JSPS core-to-core program. The group of Prof. Satoshi Hamaguchi developed a reaction-diffusion-convection simulation for the generation and transport of chemical species in water, introduced by atmospheric-pressure plasma. During my stay, I worked on a multiphase fluid model. The typical flow field of a turbulent atmospheric-pressure plasma jet in direct vicinity of a liquid was modelled by solving a k-epsilon turbulence model. A Volume-of-Fluid (VOF) method was applied for the coupled flow of gaseous and liquid phase. The simulations agree very well with experimental results in the literature. The results from the fluid flow simulations were integrated into the reaction-diffusion-convection equations to evaluate the influence of different flow regimes on the generation and transport of chemical species in the liquid.

At Bochum University, I am working as a PhD student within project B5 of the CRC 1316: *2D-plasma-liquid-solid interfaces – plasma electrolytic oxidation*. The generated results can be useful for this project in regards of chemical species generation inside of liquids. In addition, the fluid flow model is interesting for other groups working with atmospheric-pressure plasmas

(e.g. project B2: *Self-organization of sub- $\mu\text{m}$  surface structures stimulated by microplasma generated reactive species and short-pulsed laser irradiation*).

Summarizing I can say, that I had a very pleasant stay in Osaka, that I personally enjoyed a lot. The cooperation with the Hamaguchi Laboratories were very fruitful and everyone was very kind during my stay.

*Patrick Hermanns, project B5 of the CRC 1316*



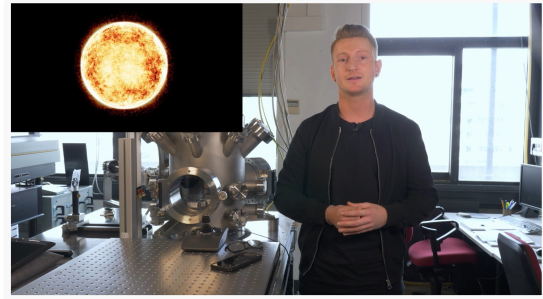
## Mobile plasma workshop for high school students finished

The last working step for the recent project of public relations is completed. The plasma truck, namely *the mobile workshop for students*, addresses physics courses within the last two years of school time.

The didactic concept of the workshop is the deepening of existing knowledge by connecting the pre-known physics with concepts from plasma physics. The concept was developed together with the research group physics didactics of Prof. Krabbe at the faculty of physics and astronomy at Ruhr-University Bochum. Within the framework of a Master thesis, Jasmin Schmidt analysed the existing knowledge of the students concerning plasmas. She found that a lot of experiments and descriptions of phenomena were treated during the classes, but have not been connected to plasmas.

Here, the workshop picks up the known experiments and categorises them in a new way. Finally, interested school classes in and around Bochum can book the

workshop for a time period of 90 minutes. On the day of the workshop, public relations staff as well as assistant students will visit the school class. A short movie has been produced to introduce the audience to the



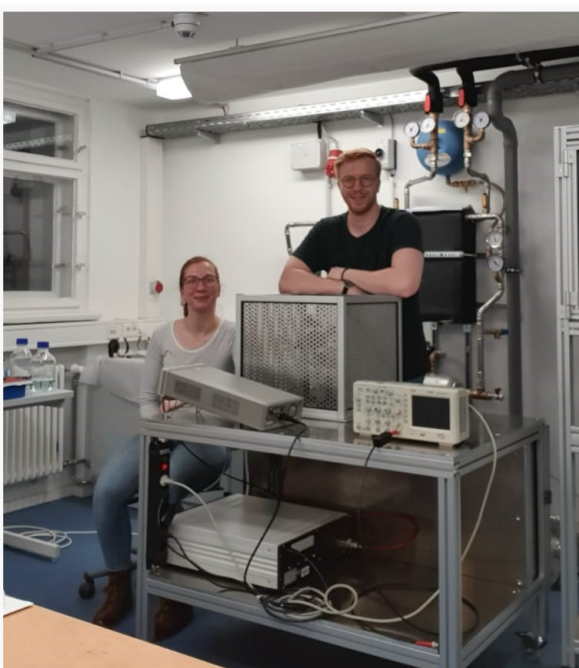
topic. Finally, the students have the chance to work on the experiments by themselves in small groups. A booklet with information on the experiments leads through the workshop. First groups might try out the workshop after the summer holidays in case that Covid-19 measures are allowing it.

*Maike Kai & Marina Prenzel, public relations CRCs*



*Successful cooperation of projects B1 & B7 of the CRC 1316*

## Setting up $\mu$ s-pulsed plasma source in liquids at FHI, Berlin



Katharina Grosse and Phillip Grosse in the FHI lab

In the framework of the cooperation between the projects B1 and B7 of the CRC 1316, the whole setup for  $\mu$ s-pulsed plasmas in liquids was transferred from Bochum to the FHI in Berlin. Afterwards, from February 17<sup>th</sup> until February 21<sup>st</sup>, 2020, PhD student Katharina Grosse from project B7 visited the group of Prof. Roldan Cuenya in Berlin to set up the experiment with the local PhD student Philipp Grosse from project B1. The cooperation between these projects should unravel the question, whether and how catalytic surfaces used for electrochemistry can be recovered by discharge treatment inside the electrolyte. With the move of the experiment from Bochum to Berlin and preliminary measurements, the first step is completed to investigate the influence of the plasma generated in-liquid species on the catalysts.

*Katharina Grosse, project B7 of the CRC 1316*



## Grand-canonical molecular dynamics to study interfacial processes: Application to the oxidation and oxygen reduction reaction on platinum surfaces

In order to better understand the interaction of plasmas with surfaces, theoretical modeling can be a powerful tool. In this respect, it is the aim of computational chemistry to resolve the relationship between structural properties and activity of the ongoing processes even on an atomistic scale. As quantum mechanical tools are limited on the time and length scale, we have developed the ReaxFF-Grand

Canonical Molecular Dynamics (GC-MD) approach allowing us to model systems in or near their steady state.

[1] In a nutshell, the algorithm allows to adjust the composition of the system continuously regarding the educts and products. Hereby, the system of interest can establish an equilibrium composition of

and the performance of this method, we applied it to the well-studied reaction of water formation on Pt(111) out of gaseous  $H_2$  and  $O_2$  molecules. We could deduce the stepped Pt(221) surface as the most active and most selective towards  $H_2O$  formation out of the investigated Pt surfaces. Another interesting point is our observation that steady state seems to be linked to

a constant  $OH^*$  coverage on the Pt surface, with  $OH^*$  being mainly stationary adsorbed.

To highlight this GCMD approach further, we performed an extensive investigation of differently shaped platinum nanoparticles aiming to allocate the active sites for  $H_2O$  production while taking into consideration surface roughening and thermally induced structural changes.[2] We

attributed the most active sites to exposed, low-coordinated sites as well as pit-shaped arrangements originating from roughening at vertices and edges.

We are looking forward to extending this method to other (electro-)catalytic systems of interest and, especially, to increase our knowledge on the effects of reaction conditions on a system's behavior and characteristics.

As oxidation of the surface turned out to play a crucial role, we also studied the process of platinum oxidation and the related effects on the degradation of platinum electrocatalysts.[3] Here, 3 nm cuboctahedral platinum nanoparticles, which are frequently used for (electro-)

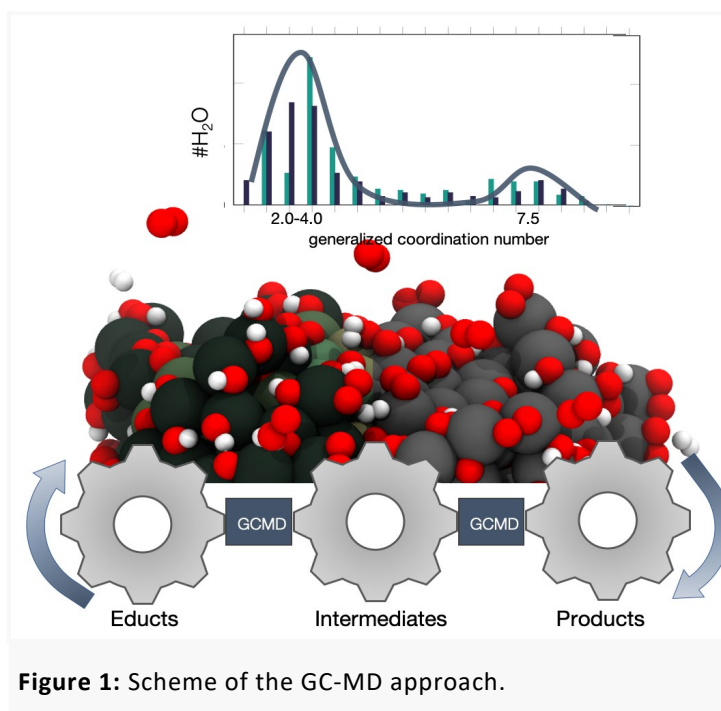


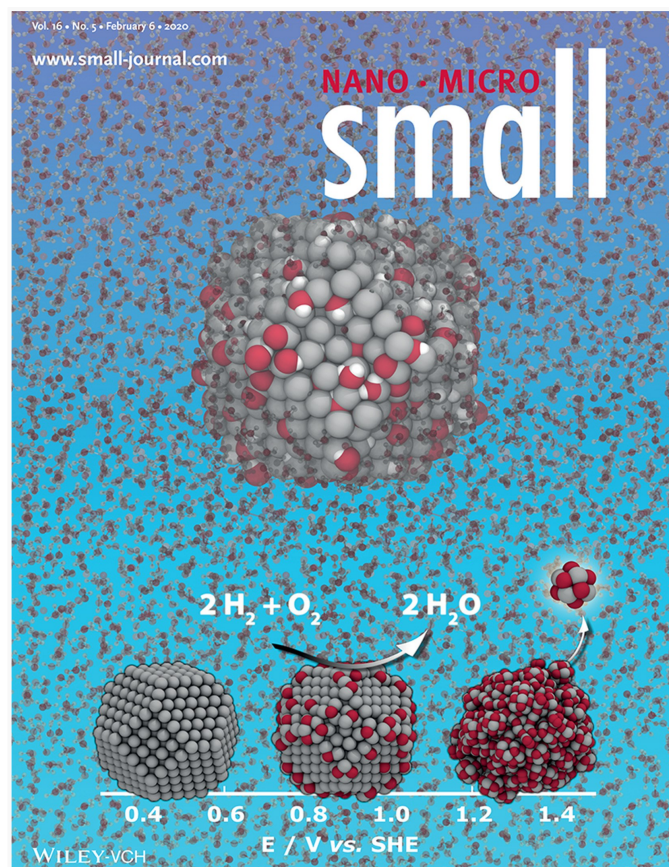
Figure 1: Scheme of the GC-MD approach.

*It is suggested that surface oxides are involved in the oxygen reduction reaction mechanism, whereas theoretical studies are often limited to studying isolated adspecies on clean crystal surfaces.*

educts, intermediates and products on the surface, but also in contact with a surrounding reservoir (which could be a plasma phase). For testing the capabilities

catalysis, were oxidized in a simulation scheme utilizing reactive force fields and a random sampling approach. Simulations revealed three distinct stages of the oxidation process: i) adsorption of oxygen atoms at reactive edges and vertices; ii) additional oxidation of the facets and increased roughening of the particle; iii) complete oxidation of the particle into subunits of  $\text{Pt}_6\text{O}_8$  stoichiometry.

These  $\text{Pt}_6\text{O}_8$  clusters were shown to be stable and hydrophilic using additional Density Functional Theory



**Figure 2:** Publication on Oxidation of Platinum Electrodes.

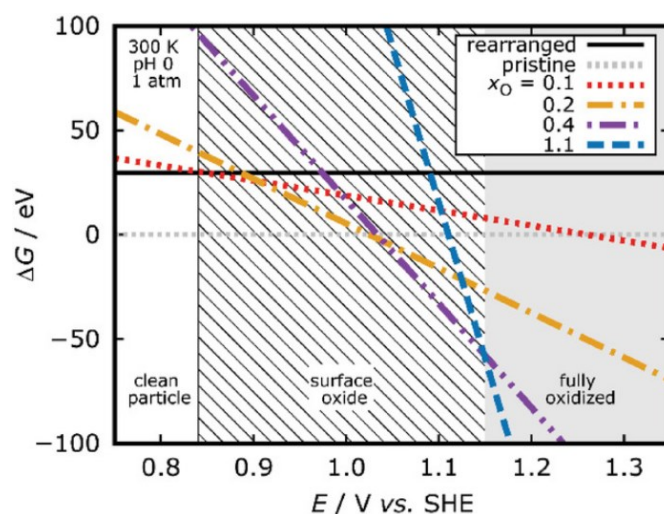
calculations. They are therefore suggested to play an important role in the oxidative degradation of platinum nanoparticle catalysts in aqueous media.

By calculating formation energy values for the generated dataset of oxidized particles and further refining the most stable structures by considering solvation and entropy contributions, an electrochemical phase diagram was constructed, see Figure 3.

The phase diagram predicts that stable surface oxides exist in a potential range for typical electrochemical

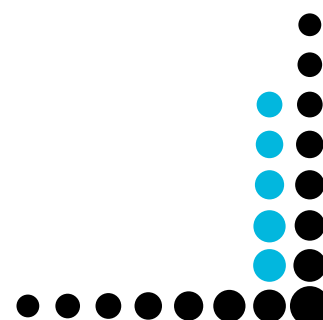
applications of oxygen reduction catalysts (0.8 V). It is therefore suggested that surface oxides are involved in the oxygen reduction reaction mechanism, whereas theoretical studies are often limited to studying isolated adspecies on clean crystal surfaces. Complete oxidation of the particle into  $\text{Pt}_6\text{O}_8$  subunits is predicted to occur at ca. 1.2 V vs. the standard hydrogen electrode (SHE), which is in agreement with experimental observations.

*Timo Jacob, project B4 of the SFB 1316*



**Figure 3:** Simulated electrochemical phase diagram for the oxidation of a 3 nm cuboctahedral Pt nanoparticle.

- [1] C. K. Jung, L. Braunwarth, T. Jacob J. Chem. Theory Comput. 2019, 15, 11, 5810–5816.
- [2] L. Braunwarth, C. K. Jung, T. Jacob (submitted) Top. Catal.
- [3] B. Kirchhoff, L. Braunwarth, C. K. Jung, H. Jónsson, D. Fantauzzi, T. Jacob, Small 2020, 16, 1905159.



## Portraits and interviews of international researchers within the CRCs

The CRCs do not only aim at national cooperation between different research institutes, but also international exchange. However, the projects are not only enriched by the cooperation with international researchers, there are also several researchers from abroad who are now working on CRC projects in Germany.

We have talked to some of them about their career and how they got to work for the CRC as well as their experiences on similarities differences of the countries they have worked in.

*interviews by Maike Kai, public relations  
for the SFB-TR 87 and CRC1316*

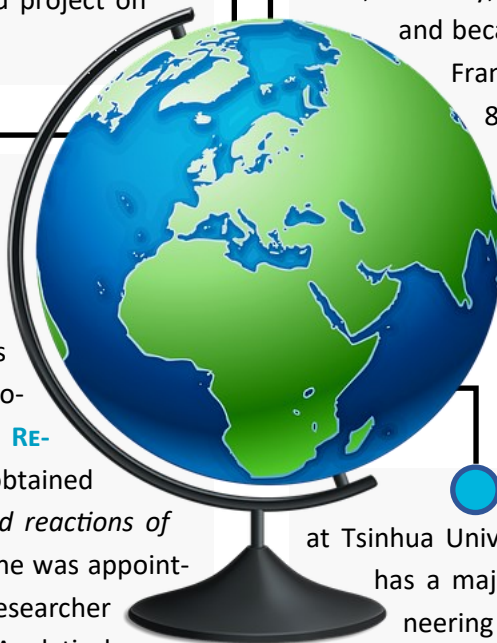
**LAURA CHAUVET** studied in **FRANCE** and did her PhD in Albi on plasmas at atmospheric pressure after doing her Master in nanoscience in Toulouse. She chose to go to Albi to allow her to be able to gain knowledge about plasma physics and analysis. After her PhD, she first worked in the laboratory for one year and collaborated with another laboratory in **SPAIN**. She then applied to EP2 in Bochum and got a position in the CRC 1316 related project on plasma chemistry.

**MATHEWS GEORGE** went to school in **INDIA** and did his Bachelor in physics in Bangalore. He then moved to Marseille, **FRANCE**, for his Master studies and has started his PhD in the SFB-TR 87 in Bochum. After his bachelor studies in India, he decided to apply for a Master in France. He then came to Bochum, Germany, for his PhD to study plasma physics and because of the advice he had gotten in France. He got to work to the SFB-TR 87 by applying to the chair of experimental physics 2 and got a topic that was included in the SFB-TR 87.

**IHOR KOROLOV** was born in **UKRAINE** and went to Sumy State University there where he obtained his Master's degree in physics/electronics. Since he prefers experimental work rather than theoretical, he moved to Prague, **CZECH REPUBLIC**, for his PhD. In 2008, he obtained his PhD on the *Recombination and reactions of ions at thermal energies*. In 2008, he was appointed as a Marie Curie Experienced Researcher (ER) within the FP6 GLADNET (Analytical Glow Discharge Network) project at Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences. From 2011 to 2016, he worked as a research fellow at MTA SZFKI and later on at the Wigner Research Centre for Physics. During his previous work in **HUNGARY**, they had a long-term collaboration with the Ruhr-University Bochum, which he has visited several times. During this collaboration he significantly expanded his research network, met a lot of very good/intelligent people and friends that helped him to find and apply for the position at the CRC 1316.

**YANJUN DU** finished her PhD study at Tsinghua University, Beijing, **CHINA**, in 2018 and has a major in power engineering and engineering thermo physics. She also spent one year at the University of Minnesota, **USA**, as a visiting graduate student during her PhD study during 2015-2016. After she received her PhD degree, she worked at Tsinghua University as a postdoc researcher for one year.

She got to work for the CRC 1316 by applying for the Alexander von Humboldt postdoc fellowship with Prof. Czarnetzki who kindly agreed to be her host. After the successfully granted the scholarship, she joined Prof. Czarnetzki's research group and got the opportunity to work within CRC 1316 in July 2019.





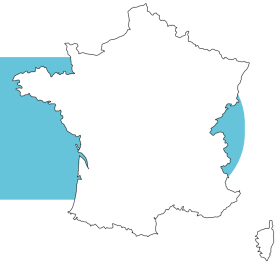
Mathews George



India — France



„The review within three months also pushes you to get forward. It is also very supporting that the projects are overlooked [...] “



**Which differences or similarities did you notice between the research abroad and in Germany?**

In France you get paid for your Master thesis if you work in the lab for more than two months. In Germany it is easy to communicate in English as most people, not only in research, speak the language. Regarding the studies in India, students do not gain much experience in the lab in contrary to Germany. In India, the possibilities to repeat exams are limited, as well as the course options at university. The quality of the courses and exams strongly depends on the university.

**What do you enjoy about working within the CRC?**

The work within the SFB-TR 87 is very organised. The review within 3 months also pushes you to get forward. It is also very supporting that the projects are overlooked and that you have a supervisor who checks the results.

**What did you enjoy about working abroad?**

It's always nice to get to know other cultures and people.

**Is there something about research abroad you would like to be implemented into the work life in Germany?**

Getting paid during the master thesis was a great financial support and from my point of view, would be nice to be implemented.



Yanjun Du



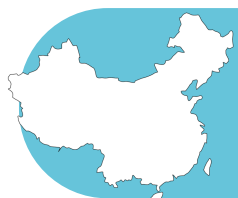
China — USA

**Which differences did you notice between the research abroad and in Germany?**

Actually, based on my personal experience, there are indeed some differences between the research in China and Germany. Firstly, for the type of projects, I have the rough feeling that there are more fundamental projects in Germany compared with China. Maybe this is also attributed to the fact that I was in the department of engineering in China while now I am in the department of physics. Most projects I participated in before were led by the industry and promoted by a specific application target. Secondly, regarding lab life, the labs in Germany are always equipped with several professional technicians, such as mechanical, electronic, and IT technicians, while in China generally the students need to do all these jobs by ourselves.

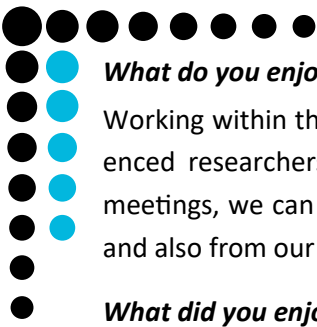
**Are there striking similarities you have noticed in research despite cultural differences?**

There are some similarities. For example, researchers in both China and Germany are pursuing high-quality research and paying much emphasis on international cooperation.



„I would speak highly of the fact that the SFB and Humboldt foundation emphases very much on gender balance. As female researcher I feel very welcomed and cared about here.“





**What do you enjoy about working within the CRC?**

Working within the CRC 1316, I got a lot of opportunities to meet and collaborate with many excellent and experienced researchers from different countries and different research areas. For example, during the regular CRC meetings, we can present our recent progress and obtain valuable guidance and comments from other colleagues and also from our Mercator fellows. In addition, we also have workshops on different topics which I also enjoy a lot.

**What did you enjoy about working abroad?**

When I was in China, I worked at Tsinghua University, which is one of the best universities and research institutions in China. Tsinghua has a very huge and beautiful campus, a good scientific research atmosphere, and excellent students to work with.

**Is there something about research abroad you would like to be implemented into the work life in Germany?**

Thanks to the rapid-growing e-commerce industry in China, when we want to machine something or fix some instruments, we can easily get contact with the manufacturers or companies via the internet. The application processes in the university are also all done online, which makes things much simpler and more efficient. For this particular point, it might be better if we can have such an efficient online system also in Germany.

**Is there something else about research abroad or in Germany you would like to mention?**

I would speak highly of the fact that the CRC 1316 and Humboldt foundation emphasizes very much on gender balance. As a female researcher I feel very welcomed and cared about here.



Ihor Korolov



Ukraine — Czech Republic — Hungary

**Which differences did you notice between the research abroad and in Germany?**

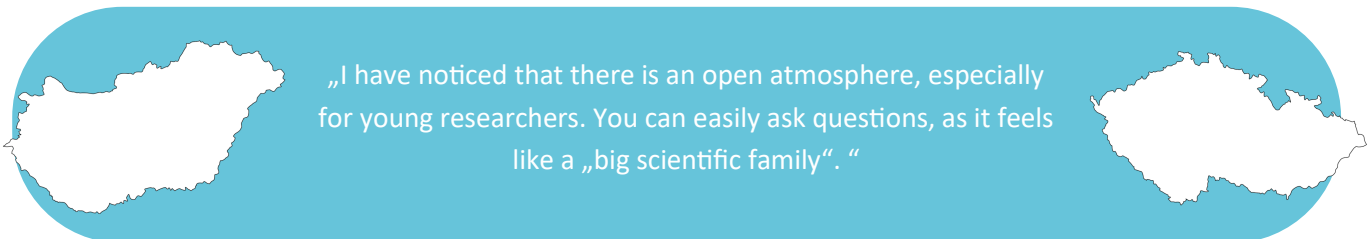
The amount of resources for projects is much higher in Germany as the government provides more funding. Also, the funding is higher.

**Are there striking similarities you have noticed in research despite cultural differences?**

I have noticed that there is an open atmosphere, especially for young researchers. You can easily ask questions, as it feels like a "big scientific family". The labs are also very similar abroad and in Germany.

**What do you enjoy about working within the CRC?**

I really see that it is a friendly, safe and protected environment where problems are solved jointly. In addition, there is an intensive knowledge transfer and a lot of exchange between the labs, as all projects should collaborate. The CRC offers the change to gain new skills, learn a new language, build a network and expand the already existing one.



„I have noticed that there is an open atmosphere, especially for young researchers. You can easily ask questions, as it feels like a „big scientific family“.“

**What did you enjoy about working abroad?**

In general, going abroad always pushes you out of your comfort zone. I have learned about the differences between the Eastern and Western European mentality, learned new languages and culture and met many new people. I have noticed, that Germans need some time to open up but then they are very friendly. Also, in Germany, students have more opportunities to go abroad due to the grants available.

**Is there something about research abroad you would like to be implemented into the work life in Germany?**

For foreigners, there are quite a few beaurocracy loops that cause some difficulties in the beginning.

**Is there something else about research abroad or in Germany you would like to mention?**

There is a very good social security system in Germany.



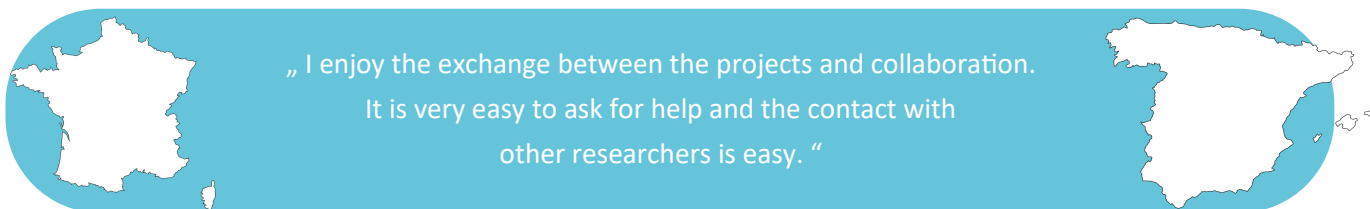
Laura Chauvet  France — Spain

**Which differences did you notice between the research abroad and in Germany?**

In Spain, it is legal to not get paid during the PhD and most thesis are worked on for about 5 years. In France on the contrary, you get paid a gratification if you work in the lab for more than two months. Compared to Germany, the thesis system in France is different. There is no Bachelor or Master thesis, but instead there are internships of different lengths with reports at the end of the internships. These are shorter than the German Master thesis though. Therefore, in France students need more time to get used to the lab during their PhD, while in Germany, students seem well prepared after writing two theses.

**Are there striking similarities you have noticed in research despite cultural differences?**

In research, there are the same overall goals. Also, there is mutual assistance between the students and international standards exist.



**What do you enjoy about working within the CRC?**

I enjoy the exchange between the projects and collaboration. It is very easy to ask for help and the contact with other researchers is easy. This allows you to get all the information and help needed. It is also nice to have input about the different projects.

**What did you enjoy about working abroad?**

In France, I was in a small lab. This meant, that everyone knew each other and the ways were very short. I believe that in a big lab it is harder to contact the supervisor. Concerning working in Germany, I wanted to see another way of organisation in research and learn new methods, as well as meet a new culture.

**Is there something about research abroad you would like to be implemented into the work life in Germany?**

In Spain, people were free in choice for their projects but due to the financial situation, it was quite hard to get funding. In Germany, the system is quite close to the French one.



The CRCs, SFB-TR 87 and CRC 1316, rely also on collaborations with international experts to reach their scientific goal. Senior scientists are invited from abroad to join the CRCs to work with the early career researchers and with the PIs in the corresponding sub projects via a Mercator fellowship. Mercator fellows support the work of the CRCs. Here, we would like to present our recent collaborators of the SFB-TR 87 and CRC 1316.

## SVETLANA STARIKOVSKAIA

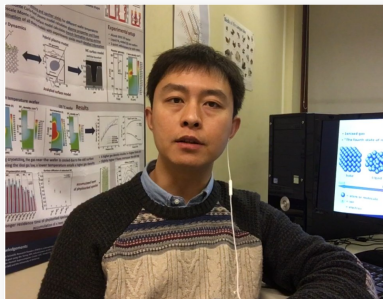


Dr. Svetlana Starikovskaia from the LPP lab at the Ecole Polytechnique in Paris joined the CRC 1316 as new Mercator Fellow. She is an expert in low temperature plasmas, pulsed nanosecond discharges, the kinetics of chemically active nonequilibrium media, the energy distribution in the discharge, the excitation of internal degrees of freedom, combustion initiation and support by nonequilibrium plasma.

Mer  
Fel

## QHAN-ZI-ZHANG

Dr. Quan-Zhi Zhang from Dalian University of Technology in China joined the CRC 1316 as new Mercator Fellow.



He is very experienced in Particle-in-cell/ Monte Carlo collision (PIC/MCC) algorithms, and simulations of plasma and plasma-surface interactions, for various applications. His research activities include the heating mechanisms and electron kinetics in DC/RF, pulse modulated, dual-frequency (EAE) capacitively coupled plasma; cryogenic plasma etching of porous materials; the propagation mechanism of plasma streamer in Dielectric Barrier Discharge and structure catalysts (like honeycomb) at atmospheric pressure.

## ZOLTÁN DONKÓ

Dr. Zoltán Donkó has been collaborating with the Ruhr University for ten years, the joint work is marked by 47 publications that appeared in leading international journals.

His recent work focuses on the kinetic simulations of high-pressure low-temperature discharges in helium and its mixtures with various gases, which directly contributes to the project A4 of the CRC 1316 (Process control in micro atmospheric pressure RF plasma jets by voltage waveform tailoring and customised boundary surfaces) and will be of relevance to other projects of the CRC 1316. His additional contributions are teaching basics of low temperature plasma science and numerical simulation techniques to researchers and students involved in the CRC, as well as acting as an external research mentor of students at RUB.

## SATOSHI HAMAGUCHI



Prof. Satoshi Hamaguchi's research focuses on plasma-material interactions in general, including their industrial applications. The aim of research is to understand fundamental mechanics of plasma-material interactions under various conditions. To achieve this, they combine plasma/beam experiments with numerical simulation/modeling. More specifically their current research topics include

- 1) etching, deposition, and surface modification processes for micro/nano electronics device manufacturing
- 2) surface modification and functionalization of biomaterials by plasmas
- 3) processing of water and biological systems by atmospheric-pressure plasmas mainly for applications in plasma medicine and plasma agriculture
- 4) dynamics and chemical reactions in plasmas under various conditions, including atmospheric-pressure plasmas.

Prof. Hamaguchi is also coordinator of the JSPS core-to-core program *Establishment of the Center for Collaborative Research in Data-Driven Plasma Science* that connects Osaka university

with Ruhr-University Bochum, and the universities in Bologna, Aix-Marseille, and York. In

the framework of this program the sending side covers international airfare and the receiving side covers maintenance and the domestic travel costs. The hosting side covers the cost of holding the seminars.



## KATHARINA STAPELMANN

Prof. Dr. Stapelmann studies the interactions of technical plasmas with biological systems on a macromolecular level. Her focus is on the characterization and optimization of plasma discharges used for biomedical applications and



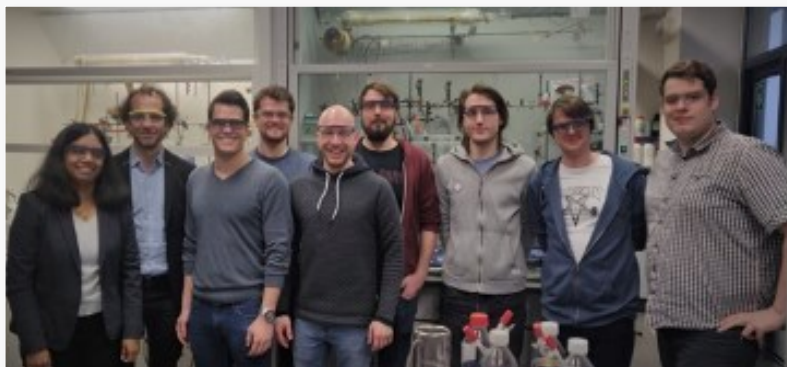
the understanding as well as the improvement of plasmas used e.g. in medicine. The applications range from wound healing to air purification, sterilization of medical instruments as well as for planetary protection purposes. Furthermore, plasma-liquid interactions and plasma discharges in liquids belong to the repertoire.

Prof. Stapelmann cooperates with the AEPT at RUB group regarding barrier discharges.



## ERWIN KESSELS

Prof. Erwin Kessels is VIP and Mercator Fellow of the SFB-TR 87 since September 2019. He joined the SFB-TR-87 workshop at RUB together with collaborators from University of Paderborn, RWTH Aachen in November 2019. His invited talk had the title *Plasma-enhanced ALD for processing at the nanoscale*.



Further, Prof. Kessels visited RUB in January 2020. He met the doctoral students of the Inorganic Materials Chemistry and visited the research group of Prof. Peter Awakowicz and Dr. habil. Julian Schulze from the Institute for Electrical Engineering and Plasma Technology.

Jan-Lucas, (joint doctoral student of Prof. Anjana Devi at RUB and Prof. Erwin Kessels at TU/e), Niklas Huster, Jean-Pierre Glauber and Florian Preischel (Master students of Prof. Anjana Devi at RUB) attended the ALD Academy Workshop that was hosted by Prof. Erwin Kessels at the Eindhoven University of Technology (TU/e) on January 14th and 15th, 2020. The focus of the workshop was atomic layer deposition (ALD) and atomic layer etching (ALE).

## Mercator Fellows

## LUDVIK MARTINU

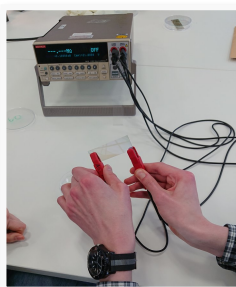
Ludvik Martinu is Professor in the Department of Engineering Physics, Polytechnique Montréal, Chairholder of the NSERC Multisectorial Industrial Research Chair in Coatings and Surface Engineering, Founder and Director of the Functional Coating and Surface Engineering Laboratory, and Co-director of the Thin Film Research Center on the Campus of the Université de Montréal. He specializes in the physics and technology of thin films, coatings, surfaces and interfaces, and is internationally recognized for his contributions to plasma processing of nanostructured materials, plasma-surface interactions, and surface engineering technologies for optical, optoelectronic, tribological, biomedical, energy, aerospace and outer space applications, and new concepts of optical coatings involving nanostructured passive and active (smart) materials. His research on coatings and thin film systems obtained by PVD and PECVD techniques has resulted in more than 350 publications and over 15 patents and patent applications.



## BO.Ing 2020

The SFB-TR 87 and CRC 1316 joined the workshop program of the Bo.Ing 2020. At the Bochum engineering forum *BO.Ing*, students from high school are given an insight into the engineering sciences in workshops, laboratory tours and discussion groups. It is aimed at interested students who would like to take up studies. Through the workshop they have the possibility to decide which study course is most suitable.

The event is organised by the zdi network IST.Bochum.NRW and is implemented in cooperation with universities from Bochum and the surrounding area. Research groups from engineering as well as from natural science present hand-on activities.



Sixteen students attended two different workshops and learned the basic ideas about plasma and its application. In hands-on activities, the girls and boys were able to perform their own experiments. Within the small groups, a lively discussion with the students took place.

We would like to thank all students from the SFB-TR 87 and CRC 1316 who helped to set up as well as dismantled the experiments during the day! The next Bo.Ing is planned for two days: March 2<sup>nd</sup> and March 3<sup>rd</sup>, 2021. We are already looking forward to the support from the different groups for the next event.

*Marina Prenzel, public relations of the CRCs*

### Recent research success

## Stable cobalt compound for atomic layer deposition

A research team from Ruhr-Universität Bochum (RUB) and Carleton University in Ottawa has manufactured a novel, highly versatile cobalt compound. The molecules of the compound are stable, extremely compact and have a low molecular weight so that they can be evaporated for the production of thin films. The team published their report in the journal *Angewandte Chemie International Edition* from May 5<sup>th</sup>, 2020.

“The few known cobalt(IV) compounds exhibit high thermal instability and are very sensitive towards air and moisture exposure. This impedes their implementation as model systems for broad reactivity studies or as precursors in material synthesis,” explains lead author David Zanders from the project B4 of the SFB-TR 87, headed by Professor Anjana Devi. In his ongoing binational PhD project, which has been agreed upon by Ruhr University and Carleton University by a Cotutelle agreement, David Zanders and his Canadian colleagues Professor Seán Barry and Goran Bačić discovered a cobalt(IV) compound that does not only possess the aforementioned properties but also exhibits an unusually high stability.

Based on theoretical studies, the researchers demonstrated that a nearly orthogonal embedding of the central cobalt atom in a tetrahedrally ar-



*© RUB, Marquard*

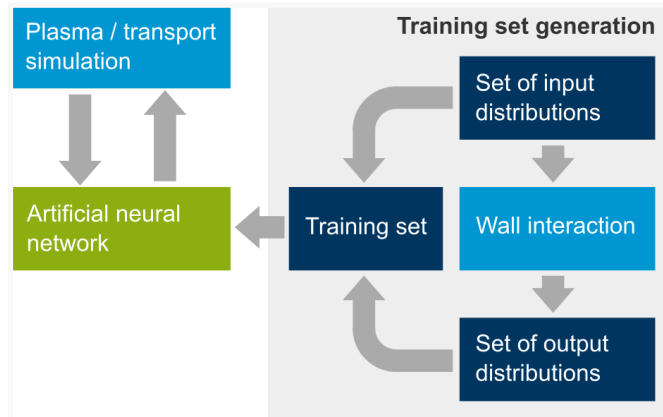
anged environment of connected atoms – so-called ligands – is the key to stabilising the compound. This specific geometric arrangement within the molecules of the new compound also enforces the unusual electron spin of the central cobalt atom. “Under these extraordinary circumstances, the spin can only be  $\frac{1}{2}$ ,” points out David Zanders. A cobalt compound with this spin state and similar geometry has not been described for almost 50 years.

Individual molecules of the compound dock onto surfaces in a controllable manner after evaporation. “Thus, the most fundamental requirement of a potential precursor for atomic layer deposition has been fulfilled,” asserts Seán Barry.

*adapted from Meike Drießen, RUB*

## Machine learning in plasma science

One of the key research questions related to high power sputter deposition plasmas investigated within SFB-TR 87 is the interaction of the plasma's energetic ions with its surrounding surfaces. The development of a consistent plasma-surface model requires a description of the surface dynamics as well as the plasma transport processes, in particular of film forming species. The length and time scales of the underlying physical phenomena of both the solid and the gas phase span orders of magnitude, rendering a consistent coupling difficult. A potential remedy for bridging the inherent scales has been demonstrated by (then) Master student Florian Krüger and co-workers of the Data Driven Modeling group at the Chair of Electrodynamics and Physical Electronics at Brandenburg Uni-



**Figure 1:** Conceptual diagram of the ANN plasma-surface interface model and the data flow for training set generation and run-time model evaluation.

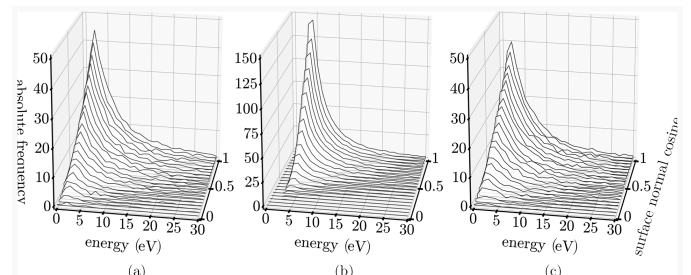
versity of Technology. The study has been published last year in the scientific journal *Plasma Sources Science and Technology*<sup>[1]</sup>. The work entitled *Machine Learning Plasma-Surface Interface for Coupling Sputtering and Gas-Phase Transport Simulations* researches the applicability of a machine learned surrogate model for high-fidelity physics regression at moderate computational cost (compare Figure 1). The proof of principle is proposed for sputtered particle distributions obtained for different energy distributions of Ar ions incident on a Ti-Al composite using TRIDYN simulations<sup>[2]</sup>. A multilayer perceptron neural network was trained and verified with a set of incident/outgoing distributions. An example distribution predicted using optimized parameters is presented in Figure 2. An error analysis was carried out for the obtained training results, assessing their quality and validity for different sets of hyperparameters. Specifically, the influence of network depth and width, activation functions, as well as regularization and early stopping is presented. It is demonstrated that the trained network is able to predict the sputtered particle distributions for unknown, arbitrarily shaped incident ion energy distributions. It is consequently argued that the trained network may be readily used as a machine learning based model interface, which is sufficiently accurate also in scenarios which have not been previously trained. Finally, the prediction time and the possibility for run-time evaluation in the frame of a Monte Carlo transport simulations are investigated.

*It is demonstrated that the trained network is able to predict the sputtered particle distributions for unknown, arbitrarily shaped incident ion energy distributions.*

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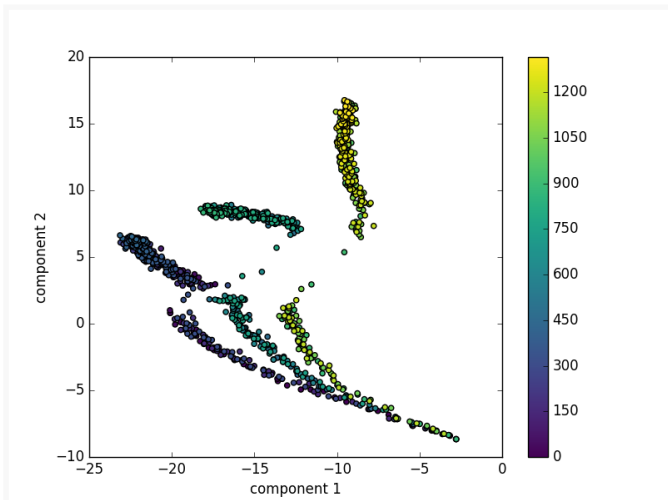
A multilayer perceptron neural network was trained and verified with a set of incident/outgoing distributions. An example distribution predicted using optimized parameters is presented in Figure 2. An error analysis was carried out for the obtained training re-

An extension of the work is currently conducted at Brandenburg University of Technology in the frame of a master thesis by Borislav Borislavov. The work entitled *Plasma-Surface Interface: Feature Extraction Using Machine Learning* deals with the unsupervised analysis of an extended set of the sputtered particle distributions. Specifically, a cluster analysis is performed based on



**Figure 2:** Predicted sputtered and reflected particle energy-angular distribution functions (a) Al, (b) Ar, (c) Ti.





**Figure 3:** 2D latent space representation of the data set of sputtered particle distributions. Colorbar indicates sample index.

convolutional autoencoders and compared to established methods such as principle component analysis. It is illustrated that, despite the nonlinear relation of the projectile and sputtered particle distributions, a significantly reduced latent parameter space is sufficient to parameterize the sputtered particle distributions for Ar

ions sputtering a binary Al-Ti composite with different chemical compositions (compare Figure 3).

Combining these results with the previously developed sputtering surrogate model will establish an even more reliable but also data-compact scale bridging. It will hence prepare the path for a comprising plasma-surface model. The conceptual methodology is envisioned also for cases with more complex surface and gas compositions encountered in reactive sputtering.

*Jan Trieschmann, project C8 of the SFB-TR 87*

- [1] F. Krüger, T. Gergs, and J. Trieschmann, *Plasma Sources Science and Technology* 28, 035002 (2019)
- [2] W. Möller and W. Eckstein, *Nuclear Instruments and Methods in Physics Research Section B* 2, 814 (1984)



*Research seminar at MCh RWTH*

## High Power Impulse Magnetron Sputtering — the age of adolescence

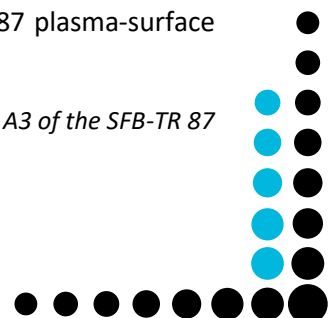
**Prof. Arutiun P. Ehasarian** from the National HIPIMS Technology Centre of Sheffield Hallam University presented a lecture on *High Power Impulse Magnetron Sputtering (HiPIMS) – The Age of Adolescence* on December 2<sup>nd</sup>, 2019.

The main focus of this seminar was on the latest findings regarding how HiPIMS processes provide turn-key solutions for many industrial applications from microelectronics to hard protective coatings. This could be obtained by a highly intense plasma which stems a wealth of reactions and discharge behaviors. This unique characteristic, hence, provides an enhanced degree of freedom and opens exceptional pathways for tailoring film properties.

Controlling the current in the discharge pulse, for instance, has been found to pave the way towards production of high density TiO<sub>2</sub> for architectural glass coatings as well as highly insulating materials such as SiO<sub>2</sub> for the semiconductor industries.

In addition, regarding the importance of adhesion in the hard-protective coatings, Prof. Ehasarian showed that HiPIMS pretreatment is capable of implanting metals and rare earth elements in the substrate while keeping the crystalline character, therefore promoting local epitaxial growth and suppressing the adhesive failure of the coatings. In another example, it has been demonstrated that the strong ionization degree of metallic species and high dissociation of nitrogen molecules in reactive HiPIMS, supplied enough ad-atom mobility on the surface and consequently enabled formation of fully dense column boundaries in TiN monolithic films having (200) preferred orientation even without utilizing substrate bias. The findings related to this seminar were profoundly in line with SFB-TR 87 plasma-surface and mechanical models.

*Soheil Karimi, project A3 of the SFB-TR 87*



## Finnish university awards Anjana Devi an honorary doctorate

Prof. Anjana Devi heads the Inorganic Materials Chemistry research group at RUB and is a principal investigator of the project B4 of the SFB-TR 87. She was recently awarded the honorary doctorate of science in technology from the Aalto University in Finland.



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Prof. Devi's research focusses on fabrication of nanostructured functional materials using gas phase routes employing new chemical precursors. Such layers are used, for example, for the production of solar cells, sensors, displays or components for micro- and optoelectronics. In recognition of her work and activities in this field of research, Anjana Devi was awarded an honorary doctorate by the Finnish Aalto University.

The key enabling technologies Devis research team works with are Atomic Layer Deposition (ALD) and Chemical Vapor Deposition (CVD). In both cases, the aim is to deposit very thin layers of a material, for example metals or semiconductor materials, on a substrate and to investigate the influence of newly developed precursors. "Anjana Devi enabled to bring the ALD and CVD communities together by organizing major international conferences and leading EU projects in this field," says the Aalto University's rationale. Since 2014, the Bochum team has had a close exchange with the Finnish university, including joint supervision of doctoral students.

*adapted from Meike Drießen, RUB*

## Upcoming events

### 29—1

**June/ July** CRC 1316—Summer Retreat  
*Rolduc — Changed into virtual meeting*

### 7—8

**July** SFB-TR 87 Project Area Meeting  
*Raefeld — Changed into virtual meeting*

### 4

**August** Hands-on Workshop 03 - Machine Learning for Materials Science and Plasma Science  
*Virtual meeting*

### 4—8

**October** 24<sup>th</sup> International School on Low-Temperature Plasma Physics: Basics and Applications  
*Online format without Master Class — more details on [plamaschool.org](http://plamaschool.org)*

### 2—3

**November** 7<sup>th</sup> International Plasma Science and Interfaces Workshop  
*RUB, organization by Hugo de Haan*

### 11

**November** SFB-TR 87 Executive board meeting

### 11

**November** SFB-TR 87 Project area B meeting  
*Bochum*

### 12—13

**November** SFB-TR 87 Project areas A and C meeting

### 16—17

**November** CRC 1316—Project Area AB meeting

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

## Research data management as central aspect within the collaborative research centres

Research data is a central output of science. They expand the scientific knowledge and are the basis for future research projects. The documentation of research data should follow subject-specific standards. The long-term archiving of research data is important for the quality assurance of any scientific work, but is also a fundamental prerequisite to allow the reusability of research results.

Researcher from the INP Greifswald enrolled a BMBF funded project with the title *Quality assurance and networking of research data in plasma technology - QPT-Dat*. This project aims to develop and test processes and methods for a quality assured and interdisciplinary reuse of research data from plasma technology.

### QPTDat cooperation

A collaboration between INP and the CRC 1316 started in 2018 and now the Research Department Plasmas with Complex Interactions, and also the SFB-TR 87 join the activities on research data management. A workshop organized by INP Greifswald in January 2020 was the starting point for further active implementations in the field of research data management in the plasma community in the CRCs as well as in the Research Department.

### First measures at EP2

As a first measure, an initiative at the research group EP2 at RUB results in an improved data storage on the local server of the institute. The storage volume has a regular backup and granting access to the complete group or to individual persons is possible. Beside measurement data, all further analysis steps are documented including meta data from all process steps. The members of the research group used a file name scheme, so that files can be found easily by other researchers.

### Research data repository

Finally, published research data can be stored and published for the open public on the repository at

[rdpcidat.rub.de](http://rdpcidat.rub.de)

The idea of such a repository is the full documentation of measurement conditions (measurement data in a

readable file format including meta data). First research groups from the CRCs have access to this repository and upload research data of published papers.

The concept of the repository is based on a multi-level system for publishing records. Users can put data online for review, which are then published by group moderators. The standards for publishing records must

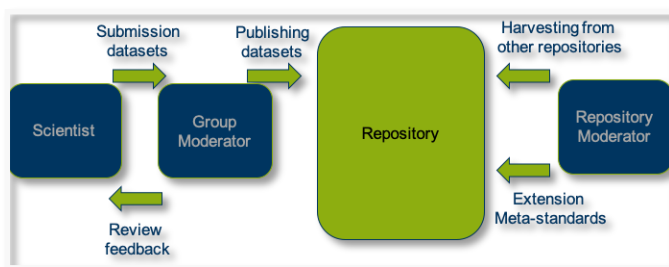


Figure 1: Scheme of publish process of data within the repository.

be defined by the group. In addition, meta data standards are currently being developed within the CRCs and together with INP Greifswald, so that data entry will be clearer and more uniform in future.

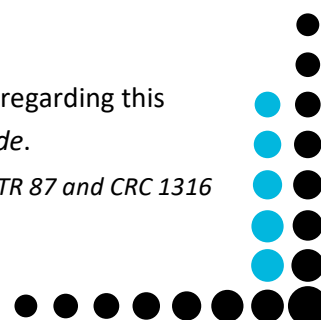
### NFDI4Phys

Recently, the Research Department Plasmas with Complex Interactions has started to join the collaboration of different scientific institutions within the so-called *NFDI4Phys* consortium. It aims to create structures and tools to simplify and unify the exchange of (mainly) numerical factual data in all areas of physics, with related disciplines and with the industry. The consortium is applying to the DFG for funding within the National Research Data Infrastructure (NFDI) project.

Within the framework of the *NFDI4Phys* consortium, the CRCs developing meta data standards for research questions in plasma science. Further goals are to contribute to the definition of basic and interdisciplinary standards and to develop methods to make research data from different sources generally accessible and interpretable.

In case, you need further information regarding this topic, please contact [rd-plasma@rub.de](mailto:rd-plasma@rub.de).

Marina Prenzel, SFB-TR 87 and CRC 1316



## Controlled atmosphere flame fusion growth of poly-oriented single crystals

Research on monocrystalline surfaces has been a hallmark for interfacial electrochemistry and electrocatalysis since the 1980's. Conducting experiments on single crystalline surfaces has allowed for the study of fundamental processes that occur on specific surface sites. This research has found that many reactions are strongly dependent on the specific surface arrangement of atoms on the electrode surface. These surface structure-activity relationships highlight the importance of fundamental research with single crystal surfaces. However, it has been very limited to noble metals, since they can be easily prepared by melting high-purity met-

(UHV) techniques.

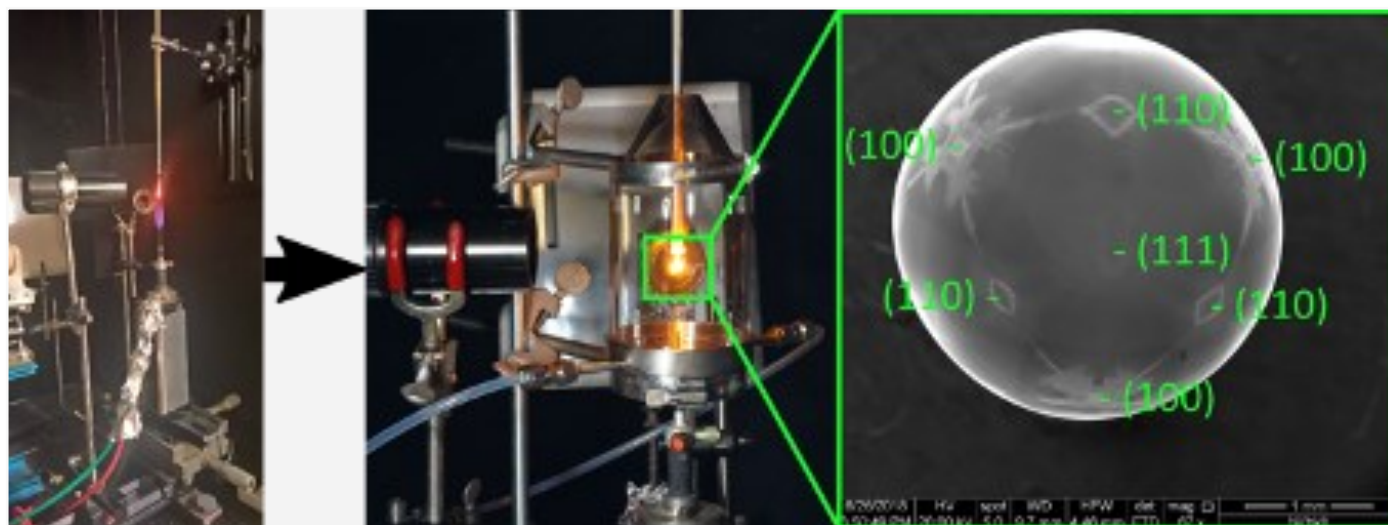
To circumvent these limitations, we have recently implemented the controlled-atmosphere flame fusion (CAFF) method, which has allowed for the first time the in-house growth of non-noble metal single crystals, without the need for complex UHV techniques.<sup>[1,2]</sup>

In Clavilier's original approach, a metal wire is melted in a hydrogen-oxygen flame using a small torch to form a liquid metal bead on the end of the wire. When the bead has been grown to the desired size, the torch is very slowly lowered away from the liquid metal droplet, causing the molten metal to begin to cool. This slow

*The CAFF method is a significant improvement of the flame fusion methodology originally developed by Clavilier and is based on two simple concepts.*

al wires in air via the "flame annealing" method developed by Clavilier in 1980, which is a flame fusion growth technique. Non-noble single crystals cannot be prepared using Clavilier's method as they will thermally oxidize. They are also very expensive and difficult to work with, since undesired oxidation or corrosion can occur while being in contact with air or electrolytes,

cooling process gives the atoms enough time and energy to arrange themselves to form a perfect, crystalline lattice, resulting in a "bead-shaped" single crystal (see Figure 1). These bead-shaped crystals are called poly-oriented single crystals (POSCs), whose surfaces have contributions from all the various low and high Miller index surfaces on the surface of the crystal (see Figure 1). Through orientation, cutting, and polishing



**Figure 1:** Progression of the traditional flame fusion method used to grow a platinum bead (left) to the CAFF method for the growth of a Ni POSC (right). The inset on the right shows an SEM magnification of a grown and slightly, thermally oxidized Ni POSC revealing the low Miller index surfaces Ni(111), Ni(100) and Ni(110).

thus damaging the expensive single crystals. Previous methods used to grow non-noble single crystals rely entirely on expensive and bulky ultra-high vacuum

one is able to prepare a monocrystalline surface with the desired surface arrangement of atoms.

The CAFF method is a significant improvement of the

flame fusion methodology originally developed by Clavilier and is based on two simple concepts. The first concept relies on a hydrogen-rich flame, where all the oxygen from the hydrogen-oxygen flame is combusted, creating a non-oxidizing flame mixture. This idea implies that any thermal oxidation that takes place must come from ambient oxygen from the air surrounding the crystal growth. The second concept can be summarized in the following question: “What would happen if one was able to control the surrounding atmosphere of the crystal growth and to expel all the ambient oxygen near the flame and growing crystal?”. By implementing a specifically designed semi-sealed chamber, which consists of a stainless-steel bottom plate with inert gas inlets and a quartz cone on top (see image), a slightly reducing environment can be adjusted inside of the

chamber. This has allowed us to grow Ni, Cu, Co and Fe POSCs for the first time with the simple and cheap flame fusion technique.

Timo Jacob, project B4 of the CRC 1316

- [1] D. Esau, F. M. Schütt, K. L. Varvaris, J. Björk, T. Jacob, G. Jerkiewicz, *Electrocatal.* 2020, 11(1), 1–13.
- [2] F. M. Schütt, D. Esua, K. L. Varvaris, S. Gemlan, J. Björk, J. Rosén, G. Jerkiewicz, T. Jacob, *Angew. Chem. Int. Ed.*, DOI: 10.1002/anie.201915389.



Cover article of the recent volume

## Journal of applied physics honours research of Sebastian Wilczek

In order to honor particularly outstanding scientific work, the cover page of each issue is highlighted with graphics by authors of an article in the current issue. The editorial office of the Journal of Applied Physics choose a cover article of Sebastian Wilczek for the recent volume.

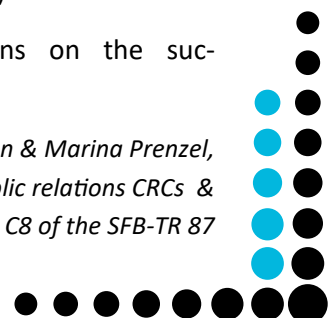
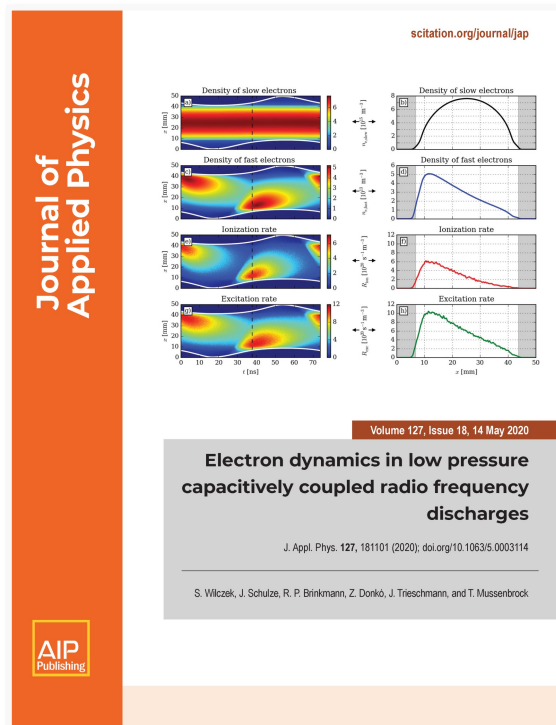
In volume 127 of the journal, the article *Electron dynamics in low pressure capacitively coupled radio frequency discharges* of Sebastian Wilczek et al. (SFB-TR 87) is published. The content of the article is the fundamental physics of electron dynamics in a low pressure electropositive argon discharge by means of particle-in-cell/Monte Carlo collisions simulations. The interplay between the fundamental plasma parameters

(densities, fields, currents, and temperatures) is explained by analysis with respect to the spatial and temporal dynamics.

This work was funded by the German Research Foundation (DFG) in the frame of the project “Electron heating in capacitive RF plasmas based on moments of the Boltzmann equation: from fundamental understanding to knowledge based process control” (No. 428942393). Support by the DFG via SFB TR 87 (No. 138690629), projects C1 and C8, SFB 1316 (No. 327886311), project A4, DFG project (No. MU 2332/6-1).

Congratulations on the success!

Jan Trieschmann & Marina Prenzel,  
public relations CRCs &  
project C8 of the SFB-TR 87



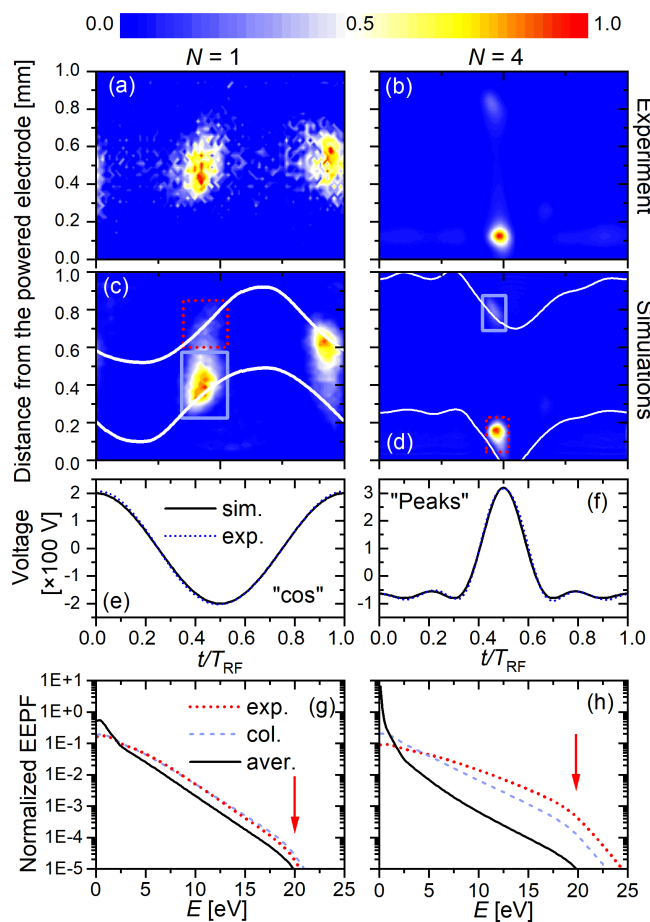
## Process control in micro atmospheric pressure RF plasma jets by voltage waveform tailoring and customised boundary surfaces

Two new papers have recently been published in project A4 of the CRC 1316: *Control of electron dynamics, radical and metastable species generation in atmospheric pressure RF plasma jets by Voltage Waveform Tailoring*<sup>[1]</sup> and *Helium metastable species generation in atmospheric pressure RF plasma jets driven by tailored voltage waveforms in mixtures of He and N<sub>2</sub>*<sup>[2]</sup>. The main motivation of this work is to demonstrate that Voltage Waveform Tailoring (VWT) in high pressure

discharges provides an opportunity to control and enhance the generation of different excited/reactive species, which are important for various applications: cancer cell/bacteria/ virus deactivation, sterilization, surface treatment/modification etc.

In collaboration with our Mercator fellow Zoltán Donkó in the first paper and based on a synergistic combination of experiments (COST-jet with phase resolved optical emission spectroscopy) and PIC/MCC simulations, we found that using ‘peaks’- and ‘valleys waveforms constructed using up to  $N = 4$  consecutive harmonics of 13.56 MHz at a fixed voltage peak-to-peak amplitude strongly affects and breaks the symmetry of the spatio-temporal dynamics of energetic electrons (Figure 1 (b) (d)) in contrast to the single frequency case (Figure 1 (a), (c)) for the He/N<sub>2</sub> mixtures. It was also demonstrated that this asymmetry can be controlled by changing the number of consecutive harmonics and the admixture of nitrogen. The simulations showed that the high energy tail of the electron energy probably function (EETF) is significantly enhanced (Figure 1 (g), (h)) during sheath collapse due to the strong asymmetry induced by VWT and, as a consequence, the generation of helium metastables and atomic nitrogen can be increased by more than one order of magnitude.

In order to experimentally confirm the above findings, since helium metastables play a key role in the chain of ion-molecular reactions in the jet, a new research was performed based on another collaboration between projects A4 and B2. The outcome of this teamwork was published in the second paper. Here, a combination of spatially resolved tunable diode-laser absorption spectroscopy measurements of the absolute helium metastable densities inside a micro atmospheric plasma jet and kinetic simulations were applied. The results obtained from the experiment and the simulations showed a very good quantitative agreement. It was demonstrated that the spatial symmetry of the helium metastable density profile can be broken and controlled via VWT (Figure 2 (a)). The peak and the gap averaged density of helium metastable was found to be significantly enhanced by increasing the number of har-



**Figure 1:** Normalized spatio-temporal plots of the electron impact excitation rate obtained experimentally (a) - (b) and from PIC/MCC simulations (c) - (d), for single frequency ( $N = 1$ ) (e) and “peaks”- voltage waveforms for  $N = 4$  (f). EETFs averaged over different spatio-temporal regions are depicted in (g) and (h).  $f_0 = 13.56$  MHz,  $\text{He} = 1000$  sccm and  $[\text{N}_2] = 0.1\%$ ,  $V_{p-p} = 400$  V

discharges provides an opportunity to control and enhance the generation of different excited/reactive species,

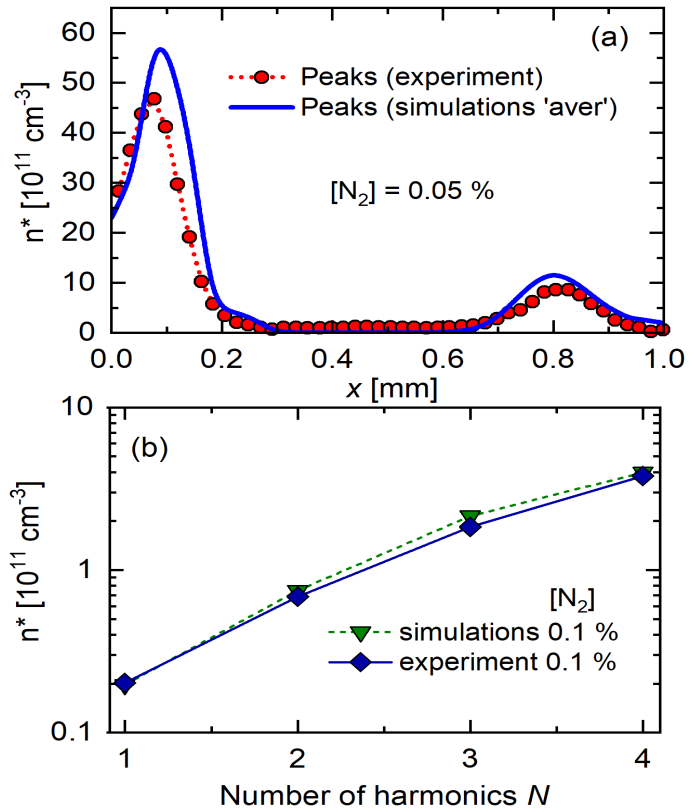
monics (Figure 2 (b)) and the peak-to-peak value of the driving voltage waveform.

Overall, the results showed that VWT allows us to control the electron driven plasma chemistry and to access regimes that were not possible to achieve with a single frequency operational mode. This is highly relevant for numerous biological and technological applications.

Ihor Korolov, project A4 of the CRC 1316

- [1] Plasma Sources Sci. Technol. 28 (2019) 094001.
- [2] J. Phys. D: Appl. Phys. 53 (2020) 185201.

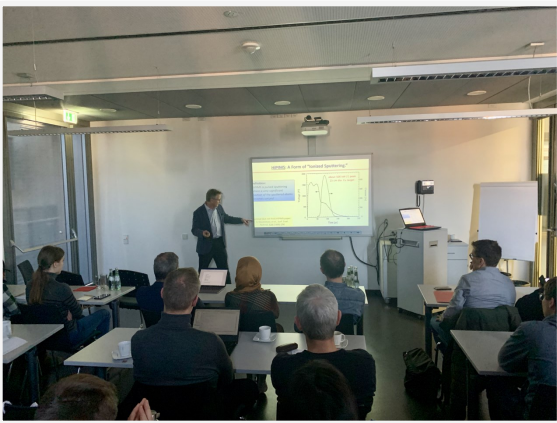
**Figure 2:** Spatially resolved absolute densities of helium metastables obtained experimentally and from simulations (a) for  $N = 4$  and  $[N_2] = 0.05\%$ . Space- and time-averaged densities of helium metastables for different numbers of harmonics and  $[N_2] = 0.1\%$  (b). The powered electrode is located at  $x = 0$ .  $f_0 = 13.56$  MHz,  $V_{p-p} = 500$  V



Research seminar at MCh RWTH

## Characterization of HiPIMS plasmas

**Prof. André Anders**, director and CEO of the Leibniz Institute of Surface Engineering in Leipzig gave a seminar on *A comparison of pulsed arc and HiPIMS plasmas* on February 5<sup>th</sup>, 2020.



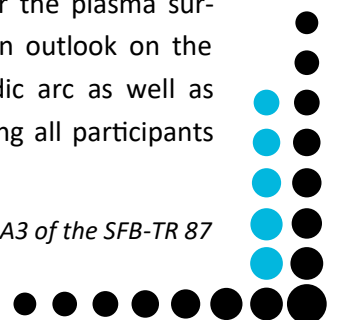
In the first part, Prof. Anders shortly presented the historical background of cathodic arc evaporation and sputtering, followed by an introduction on the physics of vacuum arcs. Thereby, the explosive electron emission was focused and this process is eventually accom-

panied by the formation of a molten pool of the target material, leading to ejection of macroparticles from the cathode. Moreover, the concept of using induction coils as filters for macroparticles in order to avoid their incorporation into the growing film was explained.

Regarding the characteristics of the vacuum arc plasma, the cohesive energy rule was discussed. The cohesive energy - required in order to transform a material from the solid state to the vapor phase - is correlated with the burning voltage of a vacuum arc and empirical laws with other material properties can be deduced. Finally, the plasma physics of cathodic arc and HPPMS plasmas were compared with emphasis on the different voltage and current characteristics.

This seminar was highly relevant for the plasma surface model within SFB-TR 87 and an outlook on the possible future directions of cathodic arc as well as HPPMS plasmas was discussed among all participants at the end of the seminar.

Marcus Hans, project A3 of the SFB-TR 87





## IMPRESSUM

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