Annual Report 2024

**Leibniz-Institut für Kristallzüchtung
im Forschungsverbund Berlin e.V.**

IKZ unifies under one roof all state-of-the-art expertise for science & technology as well as service & transfer for crystalline materials. It is this synergetic research & development approach which makes IKZ worldwide leading in crystal growth.

PROF. DR. THOMAS SCHRÖDER

Preface

Photo: Tina Merkau

Dear Readers,

the good news is: IKZ R & D programs were in 2024 overbooked by multiple interests from national & international research partners from academia as well as industry!

We carried out substantial change management over the last years, including the reorganization & modernization of our administrative & technical service units. Most importantly, IKZ initiated in its four scientific departments many new basic, applied and pre-industrial research & development (R & D) topics. The goal was to connect our unique IKZ expertise in crystal science & technology to state-of-the-art scientific & societal challenges. In 2024, we could start to harvest many prestigious fruits in the form of newly granted projects with a total volume of about 10 million €. In addition, IKZ´s R & D infrastructure mission on crystal services was strengthened with the help of administration & marketing. The IKZ crystal service is today in high demand and reached in 2024 a record annual volume of around 600,000 €. This money – the third-party funding & the crystal sales – will be of substantial importance in the following years to keep IKZ operational on a high scientific & technological level.

IKZ addresses a wide range of potential funding bodies to enable the realization of its scientific & technological goals, as highlighted by the following successful project proposals: The IKZ management is grateful to the State of Berlin for the approval of a newly funded ERDF (European Regional Development Fund) application laboratory for next generation power electronics. The application laboratory will provide an important milestone to establish IKZ as the only source in EU for 2” gallium oxide prototyping, including crystal growth, wafers & epitaxy. IKZ junior researchers were especially successful in 2024: An important success was the approval of a BMBF Nano Materials Future project to build up a Junior Research Group on innovative aluminum-gallium-oxide power transistors; further funding was awarded to Junior Research Groups in the fields of a) isotope-pure Silicon & Germanium quantum materials (DFG) and b) magneto-electric effects in hexagonal ferrite crystals for non-volatile memories (Marie Skłodowska-Curie action (MSCA) Postdoc Fellowship). IKZ Senior scientists used their (inter) national networks to participate in a number of successful calls: IKZ is a partner in the EU MSCA doctoral network “Hybrid integration of alkaline niobate-tantalate films for advanced photonic and piezoelectric devices (HINA)” and in an EU initiative to build up a technology ecosystem on optronic detector technologies. Two IKZ groups participate in the second phase of the DFG Research Unit 5044 “Periodic lowdimensional defect structures in polar oxides” (2020-2029) headed by TU Clausthal on exploring the physics & chemistry of lithium niobate-tantalate mixed volume crystals & epitaxial thin films for potential applications in quantum optics, next generation computing & 5G/6G communication. IKZ and partners were successful in a BMBF call with focus on innovative quantum materials approaches; here IKZ´s role is to grow low loss oxide crystals and provide wafers for the hybrid integration of miniaturized magnonic microwave components with superconducting circuits. IKZ technology transfer resulted in the signature of a further five years R & D contract with the Swiss company Kistler on high temperature piezoelectric langasite crystals. IKZ is active on the ramp up phase of the extraordinary item of expenditure ´Crystal Technology for Technology Sovereignty` started in 2023. It is only by these additional financial means that IKZ could build up an additional IKZ prototyping laboratory with Czochralski furnaces for oxide & fluorides. In 2024, IKZ could thus sign a further industrial prototyping contract, this time with the Berlin company CrysTec to provide small scale series of innovative oxide crystals & wafers for future ultra-low power field effect transistor technologies. Well established R & D collaborations with US partners e.g. from Cornell University are of central importance for the success of this project.

Without doubt, all these recent funding successes will help IKZ to strengthen its international leading role as EU flagship institute in the field of crystal science & technology. Challenges are given for IKZ with respect to IKZ infrastructure. The successful implementation of our IKZ strategy addressing the increasing needs in EU for trustworthy & reliable R & D on crystals for key technologies resulted in a substantial growth in staff & infrastructure. In future, IKZ´s existing building infrastructure can no longer provide neither additional technical laboratory nor further office space. Potential ideas to extend IKZ infrastructure are discussed with Land Berlin & authorities but timely solutions are not yet readily available.

With best regards

THOMAS SCHRÖDER

Content

The Institute

The Leibniz-Institut für Kristallzüchtung (IKZ)

is an international competence center for science & technology as well as service & transfer for crystalline materials. The R&D activities cover basic and applied research up to pre-industrial development.

Crystalline materials are the key to the realization of electronic and photonic solutions to social challenges. This includes artificial intelligence (communication, sensor technology, etc.), energy (renewable energies, energy conversion etc.) and health (medical diagnostics, modern surgical instruments etc.). The IKZ develops innovations in crystalline materials by combining inhouse expertise in equipment engineering, numerical simulation and crystal growth to provide highest quality crystalline materials with tailored properties.

In the future, the institute will also intensify its efforts to promote innovation by crystalline materials in cooperation with partners from technology platforms as well as industrial companies. This includes the reliable evaluation and benchmarking of innovative crystalline prototype materials for disruptive technology approaches.

The research and service tasks of the institute include:

- Development of technologies for growth, processing and characterization of bulk crystals and of crystalline structures with dimensions in the micro- and nanometer range and of comprehensive growth technologies
- Supply of crystals with non-standard specifications for research and development purposes
- Modelling and investigation of crystal growth processes
- Experimental and theoretical investigations of the influence of process parameters on crystal growth processes and crystal quality
- Development of technologies for the chemo-mechanical processing of crystalline samples and scientific investigation of related processes
- Physico-chemical characterisation of crystalline solids and development of suitable methods; investigation of the correlation between crystalline structures and properties
- Development and construction of components for growth, processing and characterization of crystals

The further materials research towards applications will drive innovations by crystalline materials:

- Crystal prototypes development for the reliable benchmarking of innovative crystals with tailored properties for key technologies in electronics and photonics
- Prototype supply of innovative crystals up to small-scale batches – with tailored properties and specifications – for reliable technology research, including preparations for market introduction
- Development of wafering processes for new materials, fine processing of special optical crystals.

Materials presently in development (examples):

- Wide band gap semiconductors (aluminium nitride, oxides) for high temperature, power- and optoelectronics
- Oxide and fluoride crystals for acousto-electronics, laser-, opto- and sensor-technology
- Silicon for power electronics
- Isotopically pure semiconductors (silicon and germanium) for quantum technology
- Gallium arsenide for wireless communication and in high-frequency technology
- Silicon/germanium-crystals for radiation detectors and diffraction gratings, crystalline Si/Ge layers for thermo-electric devices
- Ferroelectric and semiconducting oxide layers for micro- and power electronics, sensor applications or data storage

Award of the audit berufundfamilie certificate *Photo: berufundfamilie Service GmbH*

IKZ as family-friendly employer

The institute intends to create a co-operative and open working environment for all employees.

It places special emphasis on the reconcilability of job and family, offering flexible working time models as well as full or part-time employments. In 2015, the institute has been awarded the audit berufundfamilie certificate for its family-friendly human resources policy. During the following three years, we have been implementing the objectives defined in this process. The certification has been renewed in 2018, 2021 and in 2024.

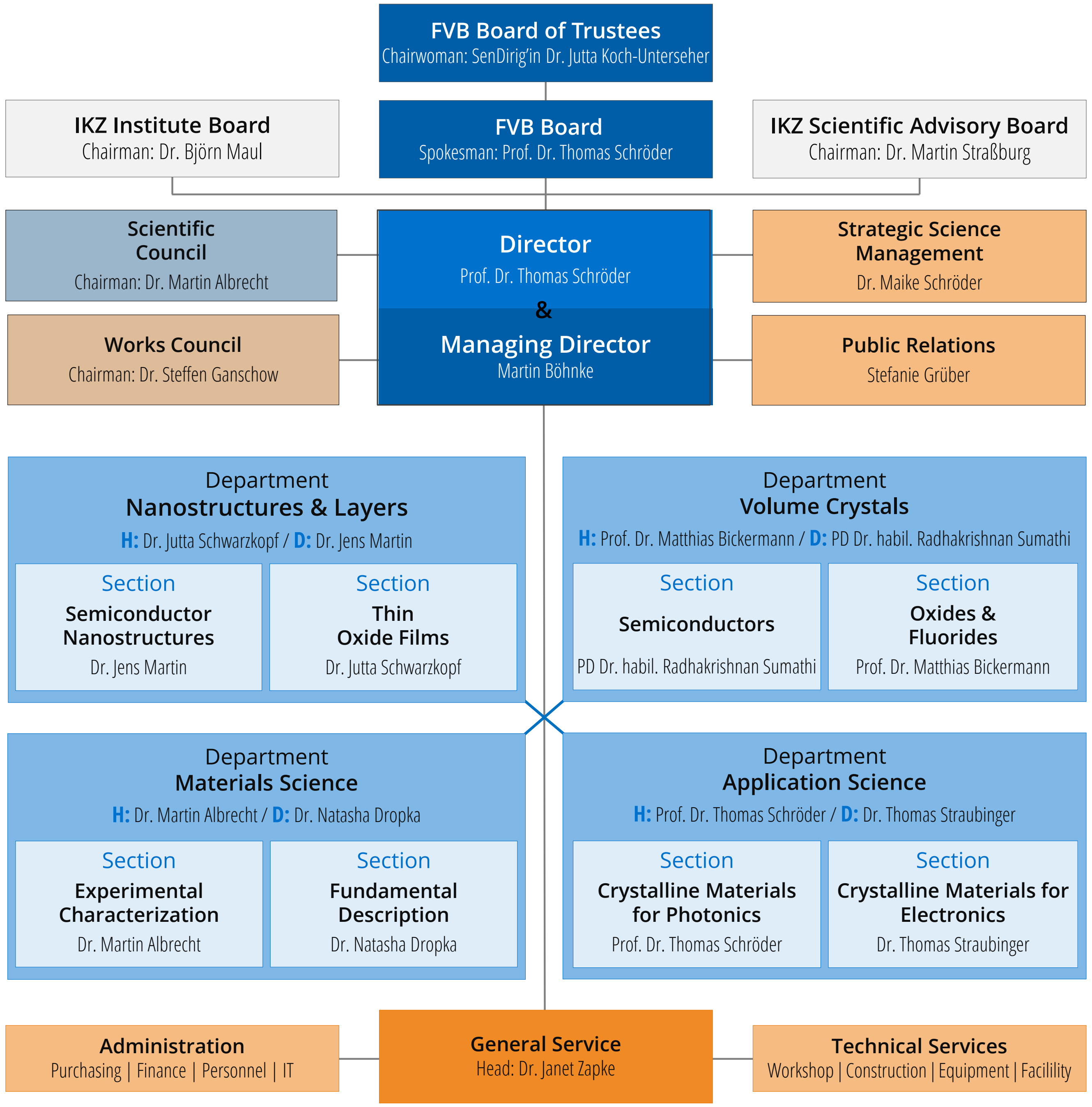
The certificate is issued under the auspices of the German Federal Minister for Families and the German Federal Economics Minister.

More information is available under **beruf-und-familie.de**

Zertifikat seit 2015
audit beruf**und**familie

Organisation chart

as of 30 June 2024



Scientific advisory board

as of 30 June 2024

Chairman

Dr. Martin Straßburg (until 31.12.2024)
ams-Osram International GmbH, Germany

Prof. Dr. Jan Ingo Flege (since 01.01.2025)
Brandenburgische Technische Universität Cottbus-Senftenberg (BTU), Germany

Deputy Chairman

Dr. Roger H.M.S. Loo
IMEC, Belgium

Members

Prof. Dr. Claudia Draxl
Humboldt-Universität zu Berlin, Germany

Prof. Dr. Marc Eichhorn
Fraunhofer IOSB, Germany

Dr. Martin M. Frank
IBM, Thomas J. Watson Research Center, USA

Dr. Benedikt Kramm
PVATepla AG, Germany

Dr. Kolja Haberland
LayTec AG, Germany

Dr. Siddha Pimputkar
Lehigh University, USA

Dipl.-Ing. Michael Rosch
Freiberger Compound Materials GmbH, Germany

Prof. Dr. Clara Saraceno
Ruhr Universität Bochum (RUB), Germany

Dr. Georg Schwalb
Siltronic AG, Germany

Prof. Dr. Thomas Südmeyer
University of Neuchâtel, Switzerland

Representative of the state of Berlin

Dr. Björn Maul
Senate Department for Higher Education and Research, Health and Long-Term Care, Berlin, Germany

Representative of the Federal Republic of Germany

Dr. Dirk Ziemann
Federal Ministry of Research, Technology and Space (BMFTR), Berlin, Germany

2024 in figures

19.6 Mio
Budget total

13.8 Mio €
Institutional funding

5.8 Mio €
Third-party funding

0.1%
EU

4.8%
Federal

10.4%
Leibniz Association

10.4%
Crystal sales / service

10.7%
Industry

20.3%
German Research Foundation (DFG)

43.3%
State Berlin (incl. ERDF)

Education
(graduated)

4
Doctoral theses

16
Bachelor's and Master's theses

Publications

110
Articles in peer-reviewed journals and book chapters

Internationalization

Staff members from
24
countries

Staff 150 total

39%
Infrastructure employees

61%
Scientific employees

Female share

36%	34%	41%
Total Staff	Scientific employees	PhD students

Contributions

83
At national and international conferences, workshops, seminars

IKZ in a nut shell … today´s status & vision for the future

What is the job of a director in a science & technology institute like IKZ?

THOMAS SCHRÖDER The job description of a director is pretty easy: Take the very expertise of the staff plus the strength of the infrastructure in the institute and bring this skill set in resonance with challenges in science & society. Like in physics: If some eigenfrequencies of two different mechanical systems match, energy interaction is strongest among them.

How do you connect to your worldwide R & D community?

THOMAS SCHRÖDER IKZ is today the EU flagship institute on science & technology as well as service & transfer on crystalline materials. IKZ scientists are on the steering boards on all international and national crystal growth networks and associations, namely the International Organization on Crystal Growth (IOCG), the European Network on Crystal Growth (ENCG) and the Deutsche Gesellschaft für Kristallwachstum & -züchtung (DGKK). Certainly, all IKZ scientists are extremely active on publishing scientific papers and networking on international conferences. We expanded our outreach activities with regular news and press releases; marketing on trade shows became in last years a further milestone to reach out for new, in particular industrial partners.

How would you describe the institute´s unique selling point?

THOMAS SCHRÖDER We host under one roof the closed added value chain to lead in science & technology of crystals: Chemical metrology for specification of materials in the growth process; thermodynamic phase diagram studies to find the process to the desired crystal phase; a wide variety of volume crystal growth techniques to make the right choice; facility and work safety management to work with high pressure and various chemicals; plant engineering and workshop to build & modify essential reactor parts; simulation, FAIR-based research data management and machine learning for cost-efficient & sustainable process development; various nanostructure & thin film deposition techniques for functionalization; state-of-the-art materials science characterization for structure, spectroscopy and transport studies; high precision crystal machining for electronics & photonics and – very important – efficient administrative processes. You see: It is a long list of different skill sets which need to be continuously developed and permanently interlinked to achieve timely success in science & technology of crystals under safe working conditions.

What are these challenges in science & society which IKZ mainly addresses today?

Understanding the world by excellence in science is at the very heart of the mission of a Leibniz-Institute. For a materials science institute like IKZ, the synthesis of new crystals to unveil the physics and chemistry in different fields of science is often an underlying pattern of our activity. In this area, IKZ was very successful in the last years to competitively apply e.g. for DFG & Leibniz Competition grants; today, more than 20 DFG projects are running at IKZ and more than 35 PhD students work with us.

Serving the world by IKZ´s research infrastructure mission is a further important pillar of IKZ´s activity for science & society. IKZ offers a unique crystal service in the EU on full cost accounting basis; potential customers from academia & industry order unique R & D crystals not available on the market. IKZ improved resources and processes to serve the communities and we achieved in 2024 an all time high of crystal sales at 600 K€.

Shaping the world by technology transfer is part of IKZ´s DNA. Today, IKZ is among the ten most successful Leibniz-institutes in technology transfer. Technology transfer is not characterized by a unique transfer format but different, customer-specific transfer channels need to be promoted. IKZ hosts the strategic science management unit with FVB centralized IP, tax and inhouse counsel contract management. IKZ coined two important branches for its technology transfer: ***Innovations in and by crystalline materials.***

Innovations in crystalline materials concern crystals well established in mass markets. These crystal processes require continuous R & D support for quality improvement, cost effectiveness etc. IKZ supports all leading crystal growth companies in Germany (e.g. Siltronic, FCM, SiCrystal, Hellma etc.) plus plant engineering companies (e.g. PVA, Nürmont, SciDre, Aixtron, Bestec, LayTec etc.) based on cooperation contracts. In case of success, research results are directly implemented to the company´s product line.

Innovations by crystalline materials concerns the R & D of innovative crystals not yet in the market but with often a potential for disruptive technologies. Here, IKZ substantially invested in R & D prototyping capacities to develop small scale series of electronic & photonic crystal components. Research partners are technology makers from industry and academic technology platforms (e.g. Leibniz & Fraunhofer) which test the crystal in the final application and feed performance results back to crystal growth; only through these feedback loops efficient progress can be made. It is in this area that IKZ start-ups can be launched and IKZ is proud to have initiated four start-up companies in the last years.

How do you envision the future role of IKZ in Germany & EU?

THOMAS SCHRÖDER Geopolitical turmoils certainly negatively affect IKZ R & D programs. After decades of fruitful interaction, partnerships with Russia completely ended since 2022 and become today more & more challenging with China. Science-averse politics in US severely restricts academic freedom and further risks to capitalize in future on academic breakthroughs by innovative technologies. In this situation, a strong international EU role in science & technology is an appealing goal. Clear commitment: IKZ wishes to actively support corresponding EU & German R & D strategies. In this respect, we took the lead for four years on the Leibniz strategy forum ´Technology Sovereignty` to coordinate Leibniz activities in this important field of innovation politics. The good news for our crystal community is that materials science & materials supply receive in general increasing political & industrial awareness. From my daily experience with companies, the need for reliable crystal R & D from a central EU source concerns electronic & photonics on an equal footing. Partnerships will require in part special collaboration formats to deal with dual use compliance. Clearly, I see the future for IKZ to act as a EU & German ´Crystal Innovation Hub of Industrial Relevance ` for electronics & photonics. We need concerted science & technology R & D programs in the form of integrated vertical application alliances – without fragmenting resources and by overcoming bureaucratic barriers.

Photo: Tina Merkau

What are main pillars to build up such a ´Crystal Innovation Hub of Industrial Relevance`?

THOMAS SCHRÖDER IKZ is heading since a few years the European Network on Crystal Growth (ENCG); we conducted a European survey on R & D activities in crystal science & technology by asking all national members about active academic & industrial players in their respective countries. The result of the survey is published online in an interactive map (https://dashboard.encg.ikz-berlin.de/encg-app/). The status analysis allows to easily define two important action points: Firstly, the need for an EU & German ´Crystal Innovation Hub of Industrial Relevance`. This research infrastructure must be able to conduct R & D in crystal diameter range of 4”-8”. Many electronic & photonic production lines run on this scale today and no technology maker will step back to smaller diameters to benefit from the disruptive potential of a new crystal platform due to cost-effectiveness. However, crystal technology upscaling is expensive and IKZ cannot build up such activities with today´s existing budgets. Secondly, the education of talented scientists & skilled engineers in the field of crystal R & D must be strengthened by various education & training formats. We observe with concern the fact that many Universities in EU & Germany close down cost-intensive crystal R & D activities. People make the difference ! We have to get young talents engaged for the fascinating world of crystals in science & technology.

Something more you would like to add ?

THOMAS SCHRÖDER Let me thank all IKZ staff for dedicated work over past years. My special thanks goes thereby to our administrative & technical services, including all colleagues in the FVB Joint Administration. Thanks!

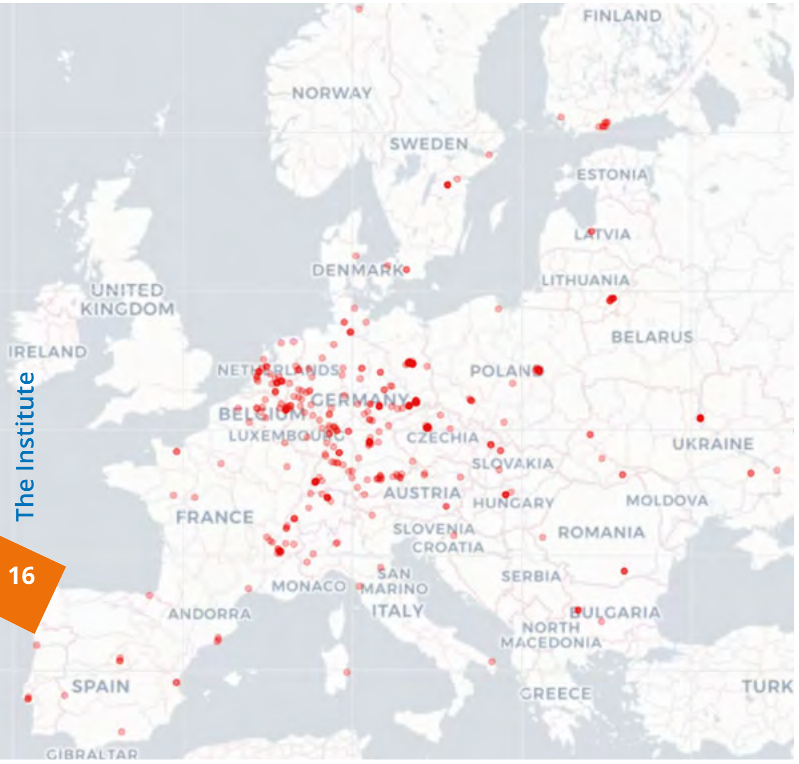
IKZ 2024

An active and dynamic year, characterized by collaborations, initiatives, and exchange with partners from science, industry, and society.

| Transfer

Status analysis on science & technology of strategic crystals in the EU

IKZ publishes an interactive map of scientific and industrial activities on crystalline materials for electronics and photonics as a contribution to the recovery of strategic competitiveness in the EU.



The application visualizes for the first time the landscape of research institutions and companies active in crystalline materials for electronics and photonics in Europe. Developed by IKZ in cooperation with the European Network on Crystal Growth (ENCG) and the German Society for Crystal Growth (DGKK), it offers a concise overview of locations and areas of expertise, supporting research, networking, and partner identification in the strategically important field of crystals.

The map enables a status analysis to be carried out on missing components and competences to re-establish strategic competitiveness and stable supply chains in the EU.

The project lays the foundation for stronger European collaboration by helping to overcome the current fragmentation into national efforts. Together with other stakeholders, ENCG, DGKK and IKZ will continue to engage with national and EU authorities on how to close the gaps in research, development and the supply of critical crystals.

dashboard.encg.ikz-berlin.de/encg-app/
encg.info
dgkk.de
ikz-berlin.de/en/transfer-service/interactive-map

| People

Martin Böhnke is the new Managing Director of the Forschungsverbund Berlin e.V.

Martin Böhnke, who has been working as a legal advisor in the joint administration of the Forschungsverbund Berlin e.V. for two years, has been appointed as the new Managing Director.

15/08/2024 He succeeds Dr. Nicole Münnich, who held the position since December 2021, following Dr. Manuela Urban and Dr. Falk Fabich.

Originally from near Hanover, Martin Böhnke most recently served as Vice President at the HAWK University of Applied Sciences and Arts Hildesheim/Holzminden/Göttingen. Prior to that, he was Chancellor of the State Academy of Fine Arts Stuttgart. After studying law and completing his legal clerkship, he held several positions at Leibniz University Hanover, including faculty director.

Commenting on his new role, Böhnke said: "The Forschungsverbund is a bold idea that creates space for excellent research in an increasingly complex, regulated environment. I'm excited to help bring this idea to life and grateful for the trust placed in me."

Martin Böhnke, Managing Director of the Forschungsverbunds Berlin e. V.
Photo: Berit Kraushaar

| Event

Science Punk: Science unleashed

What if... the lab suddenly belongs to you? No approvals, no meetings, no boss in sight – just you, your head full of ideas and all the institute's equipment at your disposal. Welcome to Science Punk, the thought experiment with a twist.

For Berlin Science Week 2024, a video was produced under the direction of Carsten Hucho from the Paul Drude Institute in Berlin, capturing exact this moment: what will happen when scientists are given total freedom? Thinking differently – crazy, visionary, maybe completely absurd. Only with one goal – to reach the one big breakthrough. The result: fictional, rebellious, inspiring – quantum computing in just one night at IKZ!

Science enthusiasts and anyone curious were able to catch the clip during the Science Week at the Tiny Gallery on Holzmarkt.

ikz-berlin.de/en/public-relations/info-for-the-media-and-public

BMBF funds the development of highly efficient β-gallium oxide heterostructures

According to estimates by the International Energy Agency, by 2050, around 90% of global energy will pass through power electronic systems. Improving efficiency by just 1% could save up to 600 TWh annually worldwide – roughly equivalent to Germany's total yearly electricity consumption.

Dr. Andreas Fiedler

Photo: Tina Merkau; Galliumoxid-Wafer (right) Volkmar Otto

The project "All-GO-HEMT" focuses on gallium oxide (Ga_2O_3), a material that enables more compact device architectures, thereby improving the efficiency of energy conversion processes and increasing system reliability. Compared to established materials, Ga_2O_3 offers promising potential that has yet to be fully realized.

The possibility of developing more efficient power electronics based on Ga_2O_3 is offset by poorer charge carrier mobility compared to established materials. "Gallium oxide behaves to its known competitors like ten meters of dirt road to one kilometer of freeway. Due to the shorter distance, your car consumes less fuel, and despite the lower speed, you reach your destination faster - all thanks to a more compact design," explains Andreas Fiedler.

Dr. Andreas Fiedler receives around €2 million for the All-GO-HEMT project

The first goal of the project is therefore to increase the Ga_2O_3 charge carrier mobility by using an innovative aluminum-alloyed heterostructure.

Andreas Fiedler emphasizes: "We are convinced that the efficiency of power electronics can be significantly increased through a combination of a more compact design and higher charge carrier mobility in our newly developed materials."

Another goal of "All-GO-HEMT" is to create a reliable material base of Ga_2O_3 and the newly developed aluminum alloy with the highest crystalline quality for research and industry. Currently, the development of high-performance, compact devices with optimized manufacturing processes is limited by the insufficient availability of high-quality material. Based on the material provided by IKZ, the project partner Ferdinand-Braun Institut (FBH) will develop advanced prototypes for power electronic components.

The industry partners involved will take on the subsequent tasks: ZF Friedrichshafen AG will assess the prototypes for their suitability in industrial application, while AIXTRON SE and Siltronic AG will analyze the entire value chain, from crystal growth to the finished device, with regard to economic and environmental sustainability.

Potentially major improvements in power electronics through the development of β-$(Al_xGa_{1-x})_2O_3/Ga_2O_3$ heterostructures in terms of efficiency, compactness, charge carrier mobility and reliability

The "All-GO-HEMT" project is being funded as part of the prestigious "BMBF NanoMatFutur" competition for young scientists and aims to establish sustainable research structures by supporting excellent young researchers. Andreas Fiedler will be given the opportunity to set up his own independent Junior Research Group at the IKZ over a period of five years – a team consisting of one postdoc and two doctoral students.

Semiconductor-based power electronics is a key technology for solving one of the biggest challenges facing society - the sustainable generation of energy. In addition to the switch to renewable and decentralized sources, the efficient use of energy is the most important lever.

With "All-GO-HEMT", we are claiming an essential component for achieving technological sovereignty in this central economic sector in Germany.

IKZ International Fellowship Award 2024 goes to Prof. Clara Saraceno

Honoring groundbreaking work in ultrafast laser systems and nonlinear optical materials

Prof. Clara Saraceno *Photo: puls 2023*

15/04/2024 The IKZ International Fellowship Award 2024, endowed with €10,000, recognizes Prof. Clara Saraceno (Ruhr University Bochum) for her outstanding research on crystal-based ultrashort-pulse solid-state lasers and their application in generating terahertz radiation through nonlinear crystals. Her pioneering work opens promising perspectives for joint projects with IKZ in the synthesis and characterization of advanced laser materials.

The award is granted for exceptional achievements in the field of oxide and fluoride dielectrics and laser crystals - materials essential for photonic applications such as laser hosts, Faraday insulators, and nonlinear frequency converters in the UV and mid-IR ranges. As part of its long-standing expertise in this field, IKZ has intensified its efforts through the establishment of the Center for Laser Materials in 2016.

The award ceremony took place during the IKZ International Fellowship Workshop on "Nonlinear Crystals for THz, Mid-IR, and UV Radiation Generation,", further promoting international exchange and collaboration.

| Event

Girls' Day at IKZ

Exploring crystals, polar bears, and smartphones – curious minds welcome!

25/04/2024 IKZ welcomed a group of curious young minds as part of the nationwide Girls' Day under the theme "A Day at the Adlershof Science and Technology Park."

No classroom, no presentations on screens – instead, protective goggles, laboratories, and crystal growth machines awaited the participants. A highlight of the visit was the tour of the crystal growth hall and the Q&A session with IKZ scientist Dr. Owen Ernst, who left no question unanswered: Why do polar bears and solar cells have more in common than one might think? How does a smartphone actually work? And is science really dry and boring? – Definitely not after this visit.

A Girls' Day that was more than just a sneak peek – it offered a crystal-clear look into a possible future.

| Event

Workshop

DGKK working group "Massive semiconductor crystals"

Meeting of the Deutsche Gesellschaft für Kristallwachtum & -züchtung (DGKK) e.V. as part of the "Berlin Photonics Days"

09-10/10/2024 Representatives from companies and institutes discussed the results of current work in the field of massive crystal growth and characterization at the working group meeting "Production and characterization of massive semiconductor crystals".

Topics included

- silicon for microelectronics and photovoltaics
- other "classic" semiconductors (germanium, III-V and II-VI compounds)
- wide band gap semiconductors (nitrides, oxides and carbides)

| Award

Advancing gallium oxide: visibility for pioneering epitaxy

Research team at IKZ honored for high-quality β-Ga_2O_3 thin films enabling next-generation power devices

Dr. Ta-Shun Chou from the Leibniz-Institut für Kristallzüchtung, awarded the DGKK Prize for Young Scientists (left, with Prof. Andreas Erb, president of the DGKK) as well as the second place in the Adlershof Falling Walls Lab 2024 (right, with Prof. Ulrich Panne, president of the Bundesanstalt für Materialforschung und -prüfung)

Photo right: Elisabeth Iglhaut, Fraunhofer IISB, Bundesanstalt für Materialforschung und -prüfung

Dr. Ta-Shun Chou, postdoctoral researcher at the Leibniz-Institut für Kristallzüchtung (IKZ), has received national recognition for research conducted within the Epitaxy of Semiconducting Gallium Oxide group, led by Dr. Andreas Popp. Their internationally acknowledged work on gallium oxide (β-Ga_2O_3) epitaxy led to major awards in 2024.

Gallium oxide at IKZ: substrates, wafers & advanced characterization

In March 2024, Dr. Chou was honored with the Young Scientist Award from the German Association for Crystal Growth (Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung, DGKK) for his key role in developing a metal-organic vapor phase epitaxy (MOVPE) process for high-quality β-Ga_2O_3 thin films. The work, including also machine learning techniques, achieved significant improvements in material quality, enabling new applications in power electronics. The award was presented at the German Crystal Growth Conference (DKT) in Erlangen.

Further visibility followed in July 2024, when Dr. Chou secured second place at the Falling Walls Lab Adlershof for his pitch "Breaking the Wall of Compound Semiconductors". Selected from 15 finalists, he was nominated for the international Falling Walls Science Summit in November 2024. His presentation highlighted the potential of gallium oxide-based semiconductors to reduce global energy losses in power conversion – a central topic of the group's long-standing research efforts.

The success builds on the group's achievements within the BMBF-funded project ForMikro-GoNext. Starting in 2020, the Popp group developed a Ga-adlayer-based growth technique for MOVPE, achieving micrometer-thick, (100)-oriented homoepitaxial β-Ga_2O_3 films with excellent electrical performance – crucial for efficient, high-power devices. Dr. Chou also contributed to the development of AI-based monitoring approaches for future industrial process control.

These results have opened commercial pathways: Since 2023, the IKZ has offered β-Ga_2O_3 substrates and epitaxial wafers grown by Czochralski and MOVPE. The group also launched the startup initiative NextGO Epi, which won the INAM AdMaLab Startup Competition in February 2024. With this, the team is actively preparing the transfer of gallium oxide technologies into industrial applications.

An interactive table invited guests to playfully explore the role of crystalline materials in everyday life.

Photo: IKZ

| Event

Where research meets the curious public: the Long Night of Science at the IKZ

Over 1000 guests visited the joint presentation of the IKZ and the Max Born Institute in Adlershof

16/07/2024 Our growth halls from the inside, laser crystals in use, lectures on technological challenges in the growth process and the social relevance of crystal availability – the program offered interesting highlights for the curious and engaged public, students, pupils, or families.

The joint presentation together with the Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy was a great success and will be continued in the future. The next Long Night of Science with IKZ participation will take place in 2026.

| Event

"Minerals – Treasures of the Earth"

IKZ and DGKK contribute to the exhibition of the Marburg Mineralogical Museum in the historic Marburg Castle (Landgrafenschloss)

21/10/2024 The Mineralogical Museum of Marburg University is hosting a two-year special exhibition, featuring highlights from 235 years of mineral collecting and exceptional pieces from the Ingrid and Reinhard Balzer Foundation. The exhibition is enriched with interactive stations and fascinating stories about minerals and rocks.

The Leibniz-Institut für Kristallzüchtung (IKZ) and the German Society for Crystal Growth (Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung, DGKK) are contributing a showcase entitled "Crystals – Key Materials for the 21st Century." It presents crystalline raw materials and illustrative graphics highlighting their role in modern technologies and everyday life. IKZ is contributing silicon and gallium arsenide crystals and wafers, along with images of crystal growth facilities from its laboratories.

Our doctoral students
Photo: IKZ

|People

Report of the doctoral students

For the doctoral students, 2024 was marked by numerous activities and the prospect of upcoming changes.

Various PhD events took place throughout the year, including our regular monthly seminars and summer barbecues. These gatherings not only provided an opportunity for professional exchange, but also for informal encounters, strengthening the sense of community among doctoral students.

At the end of the year, we organized a festive Christmas gathering with pizza and entertaining quiz games. The event provided a successful setting to celebrate the achievements of the past year and to bring the year to a close together in a relaxed atmosphere.

Group activities resumed in the summer in the form of joint barbecues and even bicycle tours. These activities in particular help to strengthen the sense of community among the PhD community and also successfully integrate new PhD candidates into the group. In general, the atmosphere among the doctoral candidates and the group cohesion within the community is very good and free of animosity, which is also reflected in the frequency of joint activities in a private setting.

A new regulation regarding the possible cancellation of the extension into a fourth year of doctoral studies was received with extremely mixed feelings, as many aspects of the communication of this plan were perceived as clearly insufficiently thought out and communicated.

Furthermore, a new lecture series was launched, known as the Career Colloquium. As part of this, doctoral graduates from professions in industry and business will be invited to the IKZ to give lectures on their professional careers after completing their doctorates. The aim is to highlight opportunities and potential career paths for IKZ doctoral students and also to create networking opportunities. These lectures are intended to show doctoral students how they can use the skills they have acquired during their doctoral studies to successfully start their careers and what career opportunities are open to them.

|Event

Workshop

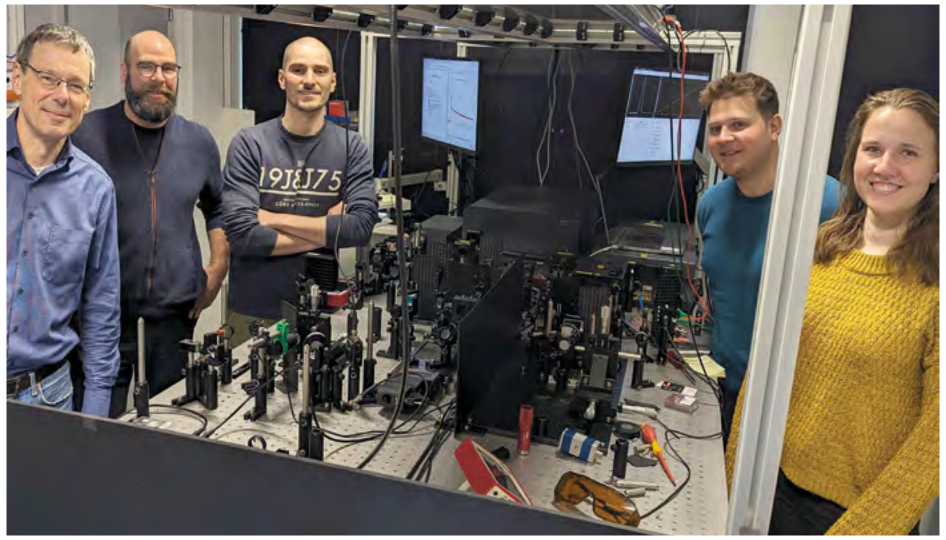
Winter School in Berlin: Materials and components for power electronics

Stakeholders from education, research and industry discussed the potential of AlN and Ga_2O_3

Participants of the 5th IKZ Winter School 2024 in Berlin on the topic "Materials Platforms and Device Technology for Power Electronics"
Photo: IKZ

04/03/2024 The Institut für Kristallzüchtung (IKZ) in Berlin and the Fraunhofer Institute for Integrated Systems and Device Technology (IISB) in Erlangen jointly organized a winter school to bring interested students and researchers together with key players from science and industry.

The forum was focused on demonstrating the potential of power electronics to significantly improve efficiency. The presentation of a technology platform for crystal growth and the respective component technology made it possible to determine the relationship between material quality and component performance.



IKZ workgroup X-Ray Optics in the new femtosecond laserlab: (left to right) Prof. Dr. Andreas Stierle (DESY Nanolab), Dr. Peter Gaal, Daniel Hensel, Daniel Schmidt, Mariana Brede (IKZ group X-Ray Optics)
Photo: Desy

|Science Infrastructure

Femtosecond laser system at the IKZ-DESY Joint Lab goes into operation

New experimental setup enables ultrafast spectroscopy studies on crystalline materials at DESY Hamburg

22/04/2024 At the Center for X-Ray Nanoscience (CXNS) at DESY Hamburg, researchers from IKZ's X-ray optics group are collaborating with Prof. Andreas Stierle's team at the DESY Nanolab to study the dynamic behavior of crystalline systems. This partnership is part of the IKZ-DESY Joint Lab.

A new femtosecond laser system for time-resolved optical spectroscopy has recently been installed, enabling the investigation of ultrafast phenomena such as high-frequency vibrations and thermal transport in crystals and nanostructures. The system allows for sampling intervals in the micro- and millisecond range with a time resolution of under 300 femtoseconds (1 fs = 10^{-15}s).

Initial experiments on InP nanocrystals have already revealed natural vibrations at frequencies up to 50 GHz. The new setup significantly enhances the Joint Lab's capabilities for advanced material characterization.

Spin-off companies

Our start-ups: transferring materials science into market-ready technologies

Glaide Data GmbH

is a spin-off company from IKZ, established in collaboration with Humboldt University Berlin (HU Berlin) within the framework of the FAIRmat project.

Glaide Data combines advanced research data management (RDM) solutions with the power of artificial intelligence (AI) and machine learning (ML). Built upon the NOMAD Oasis platform, the company provides innovative data management services, allowing researchers to concentrate on scientific innovation by managing their data complexity effectively.

NOMAD Oasis is an open-source RDM platform (www.nomad-lab.eu), developed within the FAIRmat project (www.fairmat-nfdi.eu). It adheres to the FAIR (Findable, Accessible, Interoperable, Reusable) principles, ensuring data is inherently AI-ready. NOMAD's comprehensive data model efficiently manages research data from computational studies and experimental workflows. Glaide Data's specialized services include consulting to optimize research data strategies, customized implementation of NOMAD Oasis tailored to organizational workflows, and secure, fully supported cloud hosting solutions.

Founded in 2025 by Sebastian Brückner, who leads digitization efforts in research data management at IKZ and coordinates synthesis data activities within FAIRmat, Glaide Data aims to broaden the adoption of NOMAD Oasis within the materials science community and extend its capabilities to other research disciplines. The dedicated team comprises scientists, engineers, software developers, and data specialists with extensive expertise in research data management, machine learning, artificial intelligence, FAIR data principles, and laboratory automation.

glaidedata.com

Dr. Sebastian Brückner holds a doctorate in physics and over 16 years of experience in applied materials science. At IKZ, he leads the data science team and coordinates the FAIRmat activities on synthesis data. With Glaide Data, he aims to promote NOMAD and help researchers in leveraging AI, machine learning, and lab automation for more efficient and innovative work.

TXproducts

is a spin-off from the X-Ray Optics group at IKZ and was founded in close cooperation with DESY in Hamburg in April 2021. IKZ and DESY also bundle and coordinate their activities in an IKZ-DESY Joint Lab on the DESY campus in Hamburg Bahrenfeld. The startup is also supported by IKZ's ERDF application laboratory "Materials for Oxide Electronics".

TXproducts develops and commercializes active X-ray optics for adapting the time structure of synchrotron radiation specifically for experiments at large-scale research facilities. This includes in particular the WaveGate Pulse-Picker – a compact device for selecting on-demand X-ray pulse pattern. By adapting the time structure, experiments at synchrotrons can be carried out with increased efficiency up to hundred times faster.

The technology behind the innovations from TXproducts was developed to market readiness by the founders together with a team of scientists from IKZ and various other research institutions. In particular, the IKZ provides tailor-made materials which allow efficient manipulation of X-ray pulses.

TXproducts is currently developing applications of its products in several pilot projects at the synchrotron sources DESY (Hamburg) and ESRF (Grenoble, France). For the construction of a universally applicable demonstrator, TXproducts was awarded the InnoRampUp funding from the Hamburg Investment and Development Bank IFB in October 2021.

txproducts.de

Daniel Schmidt holds a master's degree in nanoscience and specializes in time-resolved synchrotron and laser applications. Together with Peter Gaal, he is the founder of TXP and drives active X-ray optics from prototyping to market.

Dr. Peter Gaal holds a doctorate in experimental physics with a strong background in structural dynamics and solid state physics. As a researcher, university lecturer and entrepreneur, he is driving the development of active X-ray optics.

quantum grade materials [qgm] i.G.

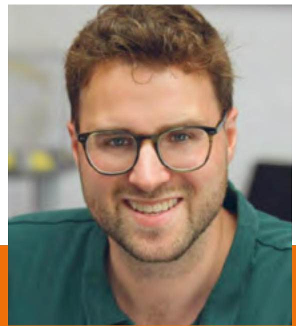
brings the future raw materials made in Lausitz to market maturity. These materials are isotopically pure semiconductors and semiconductor precursors such as silicon-28/silane-28 and germanium-73d/germane-73d. These materials are required for the production of 2nd generation quantum technologies, e.g. quantum computers, but also for other technologies in X-ray optics and cryogenics. The aim is to ensure a sustainable supply of these key strategic materials for industry and research in Europe and beyond.

The business idea was developed as part of research into SiGe heterostructures for quantum computers in the Semiconductor Nanostructures section at the IKZ. In order to guarantee the infrastructural and safety requirements for the chemical synthesis processes, the founding project moved to the Brandenburg University of Technology Cottbus-Senftenberg in 2024. The team continues to receive support from the IKZ, for example in the form of networking or expertise in volume crystal growth.

The project was awarded the Lusatian Business Start-up Prize in 2023. In 2024, funding of over EUR 900,000 was obtained through an EXIST research transfer. The start-up is scheduled to be founded in early 2026.

quantumgradematerials.de
linkedin.com/showcase/quantum-grade-materials-btu/

Dr. Owen C. Ernst
holds a doctorate in physical chemistry. He uses his experience in the fields of thermodynamics, inorganic chemistry and semiconductor physics to drive the start-up project forward. In addition to his scientific and entrepreneurial activities, he is passionate about communicating science to the public.



Dr.-Ing. David Uebel
holds a doctorate in materials science. Already during his doctoral studies, he worked extensively on the deposition of classical semiconductors. During his postdoctoral period at the IKZ, David Uebel was responsible for technology transfer and acquired a broad knowledge of the market for (isotopically pure) silicon.

Anne Handschick-Ernst
is trained in office management and has a Bachelor's degree in European Media Studies. She has already worked in start-ups and in global corporate groups. She enriches the start-up project with her commercial expertise and her experience with companies in various stages of development.

Roman Brendler
holds a diploma in physics (equivalent to a Master's degree). He gained professional experience as a programmer before founding the company Jointech e. G. as part of a team. He was a member of the board for three years and responsible for product development, new customer acquisition and the eight-strong team.

NextGO Epi

is a spin-off which aims to supply high-quality and large-scale gallium oxide (Ga_2O_3) epitaxial wafers using Metalorganic Vapor Phase Epitaxy (MOVPE), building upon IKZ's decade-long research advancements in Ga_2O_3 materials. The technology driving NextGO Epi's innovations was brought to market readiness by its founders, building on the expertise of a team of experienced scientists at IKZ. The institute also provides the essential infrastructure for the start-up, supporting this development.

The unique advantages of Ga_2O_3, recognized as a fourth-generation ultra-wide bandgap semiconductor material, lie primarily in its potentially significant cost and performance benefits over conventional power semiconductors such as SiC and GaN.

As a key innovator in Europe, NextGO Epi is focused on enabling next-generation high-power electronics by providing advanced tailored Ga_2O_3 epi-wafers that will allow device manufacturers to produce devices that are cheaper, more compact, and more efficient and even enter new areas of application beyond 10 kV. With deep expertise in epitaxial growth, AI-assisted process optimization, and market access, NextGO Epi plays a crucial role in bridging cutting-edge material innovation with industrial-scale adoption.

NextGO Epi is on the roadmap to delivering high-quality and large-size Ga_2O_3 epiwafers to customers worldwide.

nextgoepi.com
linkedin.com/company/nextgoepi/

Dr. Ta-Shun Chou
holds a doctorate in chemistry, specializing in crystal growth theory and artificial intelligence. He performed his Ph.D. study in IKZ from 2020 to 2023. His thesis presents key breakthroughs in growing high-quality Ga_2O_3 epiwafer.As a scientist-turned-entrepreneur, he is driven by a mission to bridge the gap between research and industry, accelerating the commercialization of Ga_2O_3 for next-generation technologies.

Dr. Andreas Fiedler
is an experimental physicist with a focus on semiconductor physics and devices. As the leader of the BMBF NanoMatFutur Junior Research Group All-GO-HEMT, he has in-depth knowledge in the fields of electrical engineering, advanced materials characterization, processing, and synthesis. He has been working in Ga_2O_3 research for over a decade and brings all his experience to NextGO Epi with the firm intention of transferring his scientific achievements into a real-world application and making them accessible to society.

Dr. Andreas Popp
studied physics and obtained his doctorate in 2017. At IKZ, he is the head of the research group "Epitaxy of Semiconducting Gallium Oxide," dedicated to material development for power electronics. With its work on MOVPE-based epitaxial deposition of gallium oxide thin films, the group has gained international recognition. He aims to advance materials research with a focus on developing technological solutions to address key societal challenges.

Crossing borders

Research visits by IKZ doctoral students to national and international partner laboratories

(Inter)-national research stays open up valuable opportunities for doctoral students to engage in scientific exchange and expand their expertise. Maximilian Oezkent and Christian Rhode, both doctoral students at the IKZ, were able to gain decisive impulses for their scientific work through their stays at renowned research institutions.

Maximilian Oezkent *Photo: IKZ*

Maximilian Oezkent

Maximilian Oezkent, had the opportunity to conduct research at the Polytechnique Montréal as part of a sponsored stay. This stay was made possible by a grant from the European COST Action OPERA (CA-20116) as part of the Short-Term Scientific Missions (STSM) program. During his stay, he analyzed ultra-pure, isotope-enriched $^{76}Ge/^{28}Si^{76}Ge$ heterostructures with atomic precision, a topic of great importance for the further development of quantum technologies. At the university, Maximilian Oezkent gained hands-on experience at a state-of-the-art atom probe microscope (Cameca INVIZO 6000). Quantum grade $^{76}Ge/^{28}Si^{76}Ge$ thin-film heterostructures, which were grown at the IKZ using molecular beam epitaxy (MBE), were studied by applying atom probe tomography (APT). Using this high-resolution method, he was able to map the structures and interfaces of the materials in 3D at atomic scale, which provided crucial insights into their quality and impurity content, parameters that are of great importance for the realization of quantum devices.

The stay at Prof. Oussama Moutanabbir's group at the Polytechnique Montréal enabled Mr. Oezkent to gain valuable new insights that will be included in an upcoming publication. This international collaboration underlines the importance of exchange and cooperation for the advancement of research in the field of SiGe quantum materials.

Christian Rhode *Photo: IKZ*

Christian Rhode

Christian Rhode, was given the opportunity to conduct research as a visiting scientist in the group of Prof. Dr. Thorsten M. Gesing at the University of Bremen. The focus of his research was on analyzing the crystal structure of Mg- and Zr-substituted $SrGa_{12}O_{19}$ and $Sr(Ga,Al)_{12}O_{19}$ crystals. These materials are of particular interest as they can be used as substrates for the epitaxial growth of $BaFe_{12}O_{19}$ thin films. The change in the lattice parameter associated with the chemical alteration of the solid solution allows for targeted strain engineering at the interface between the substrate and the grown thin film. This enables precise control of the ferroelectric moment of the hexaferrite.

Through the single-crystal X-ray diffraction experiments, Mr. Rhode was able to gain valuable information about the positions of the substituents Al, Mg and Zr in the crystal structure. The results contribute to a better understanding of the structural properties of the grown materials and thus make a decisive contribution to understanding the material system at a structural level. In addition to the immediate scientific interest, the insights gained are extremely relevant when evaluating the success of the growing process and also provide a starting point for further efforts to chemically alter the material. The latter in particular aims at elucidating possibilities for the adjustment of a target lattice parameter by chemical means. In addition, Christian Rhode expanded his knowledge of single-crystal diffraction and was able to make significant progress in his doctoral thesis. The research stay was made possible by the financial support of the MAPEX Core Facility.

The research stays of Maximilian Oezkent and Christian Rhode show how important national and international cooperation is for scientific development and exchange. By working closely with renowned research institutions in Canada and Germany, both doctoral students were able to significantly advance their research projects and acquire valuable methodological and theoretical knowledge that is of central importance for their dissertations and the further development of their specialist areas. This experience is not only of great importance for the careers of the doctoral students, but also contributes to the international networking of the IKZ.

From algorithms to crystal growth: A new chapter in process innovation

After a successful academic journey in Serbia and seven years of applied AI research in Berlin, Milena joined IKZ in 2024 to lead a new Junior Research Group. Her mission: to bring advanced machine learning and optimization into the world of crystal growth. In this interview, Milena shares how her background in systems and data science is shaping experimental processes, how she's building bridges across disciplines, and why leadership, like crystal growth, requires just the right conditions. She also reflects on her first year at IKZ – and why the future looks bright, structured, and full of possibilities.

| Interview

How did your academic and professional background lead you to IKZ?

MILENA PETKOVIĆ I completed both my master's and PhD studies at the Faculty of Technical Sciences in Novi Sad, where I focused on optimization and process control. I then worked as an assistant professor, driven by a strong interest in how mathematical thinking can be applied to real-world systems.

In 2017, I moved to Berlin and began working in applied mathematics and machine learning, especially on forecasting and modeling in the energy sector. Over time, my interest evolved: I wanted to bring AI not only into numerical modeling, but into direct interaction with physical processes. And when the opportunity at IKZ came, it felt like the perfect next step.

How and when did crystals trigger your interest? Have you always been into physics?

MILENA PETKOVIĆ Physics wasn't my academic home originally – my background was in systems, algorithms, and optimization. But when I encountered the world of crystal growth, something clicked. Here was a field full of complexity, precision, and physical beauty, and also full of unanswered questions perfectly suited for AI.

What drew me in wasn't just the science of crystals, it was the possibility of bridging domains. Crystals grow under strict physical laws, but we can influence them through data, models, and smart control. That's where I saw room to contribute, and to grow.

What does leadership mean to you as a scientist? (What does it mean to you to lead a team in a scientific environment?)

MILENA PETKOVIĆ For me, leading a research group is not just part of the job – it's a way to shape how science is done and how people grow within it. I don't see leadership as a matter of control or hierarchy, but as a way to empower others. My goal is to create a space where learning, innovation, and collaboration happen naturally – a place where ideas can evolve, be challenged, and take shape together.

Research, at its heart, is creative work. Leading a team means nurturing that creativity by building an atmosphere of trust, encouraging open dialogue, and sharing responsibility for both challenges and breakthroughs. I enjoy setting a strategic direction, supporting younger scientists as they grow, and connecting people across disciplines to spark new insights.

Some of the most fulfilling moments are when someone on the team comes up with a question or a solution I hadn't thought of. Those moments remind me why I love what I do.

At home, life is just as dynamic. As a mother of triplets, I've learned a lot about patience, resilience, and balancing many moving parts – lessons that often translate directly into leadership. In both science and life, I believe the best way forward is to stay curious, stay open, and grow together.

| Vita

Dr. Milena Petković

Master's and PhD in Electrical Engineering and Computer Sciences at the Faculty of Technical Sciences, University of Novi Sad. Former Assistant Professor in Serbia, focused on mathematical modeling, optimization and control.

Moved to Berlin in 2017 and worked in applied mathematics and AI, especially in predictive methods in energy systems. Since 2024 Junior Research Group Leader at IKZ, applying machine learning and optimization to crystal growth.

Research interests include multi-objective optimization, AI-driven process modeling, and digital twins for experimental systems.
Combines deep technical expertise with a passion for interdisciplinary teamwork and mentoring.

Committed to fostering inclusive research environments and supporting women in science.

Lives in Berlin with her family.
Believes that structure enables creativity – in science, in leadership, and in life.

What are you working on now? What is the benefit to society?

MILENA PETKOVIĆ Right now, my team focuses on AI-driven optimization and process modeling for crystal growth. One of the most exciting topics we're working on is transfer learning – using models trained on one material or process to support decision-making in others.

This is especially valuable in crystal growth, where experiments are slow, data is limited, and outcomes are sensitive to subtle changes. By enabling smarter predictions with less data, we can accelerate discovery, reduce energy use, and make processes more robust.

This has direct societal impact in areas like UV-LEDs, semiconductor manufacturing, or quantum technologies. Improving how crystals are grown means improving the technologies that rely on them.

What matters most to you in your research?

MILENA PETKOVIĆ For me, research is most powerful when it connects – across disciplines, across people, and across ideas. I care deeply about building bridges between digital tools and physical processes, but also between people, between senior scientists and students, between fields that don't always talk to each other.

And I care about creating space for women and diverse voices in science. I've always felt supported and respected here at IKZ and in Berlin, and I want to help ensure others feel the same. Science thrives on diversity – of thought, of background, of experience.

Outside the lab, I live a parallel adventure as the mother of triplets. It's chaotic, energizing, and teaches me things every day about patience, adaptability, and the value of small wins. That energy flows back into my work.

Your first year at IKZ – how would you sum it up?

MILENA PETKOVIĆ It's been a year of arrival, not just at a new workplace, but in a new field, a new role, and a new chapter. From day one, I've received strong support and encouragement from colleagues across the institute. There's been real openness to collaboration, to new ideas, and to integrating AI in crystal growth.

My goal now is to keep building on that, to contribute not just methods, but mindset. High-quality crystals grow under carefully tuned conditions. So do great teams, and so do successful careers. And at IKZ, I feel like the conditions are just right to grow something excellent – together.

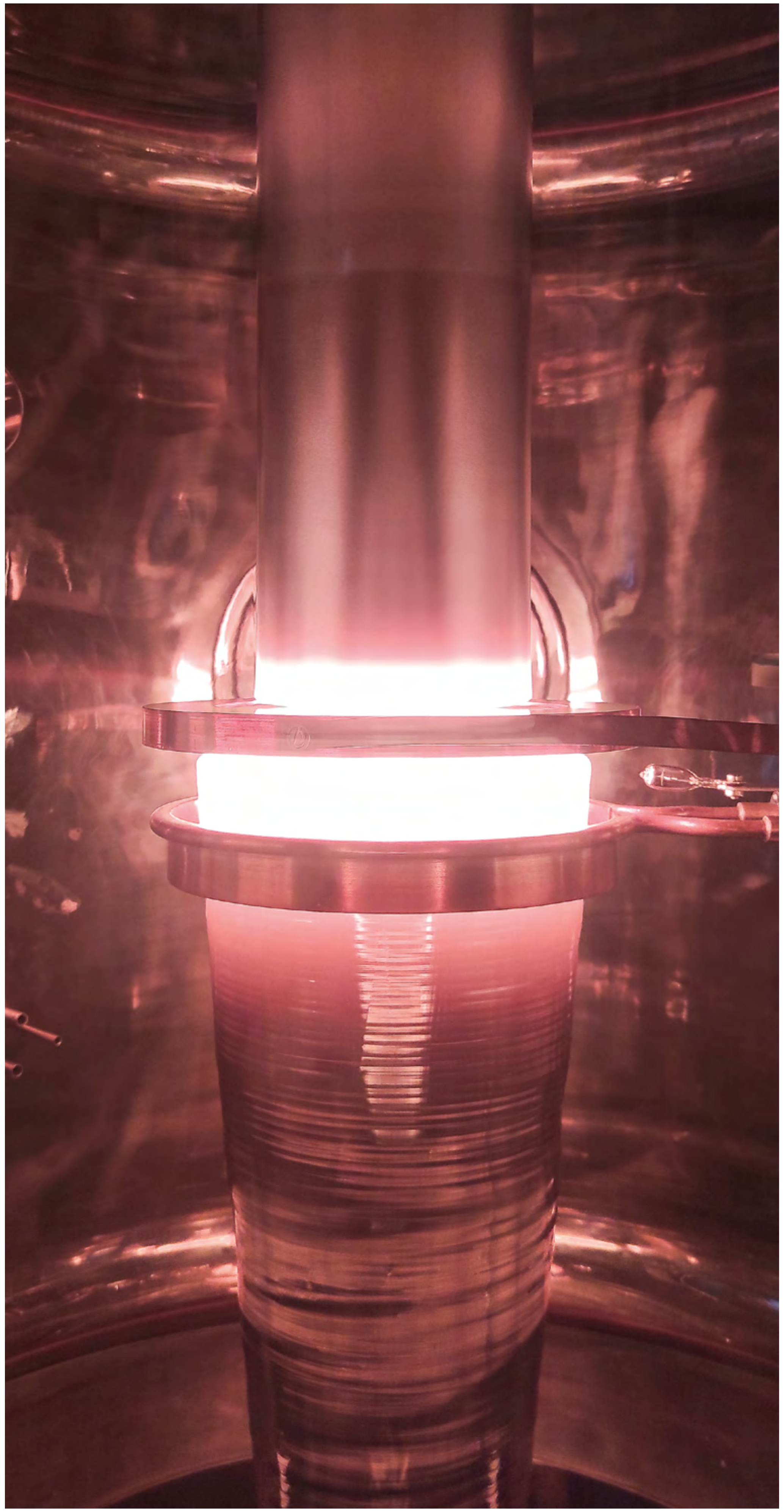


Fig. 1
The growth of an FZ-Si crystal with large diameter of 180 mm at IKZ
Photo: IKZ

Float-Zone Silicon Crystal Growth for Applications in Power Electronics and for Fundamental Research Projects such as the Einstein Telescope

At the IKZ, ultra-pure silicon crystals are grown by the float-zone method, serving as key materials for next-generation gravitational-wave detectors like the Einstein Telescope, as well as for advanced power electronics

| **Project**

FZ-Si for Power Devices

The Float-Zone (FZ) method is the only industrially established crystal growth method capable of producing ultrapure silicon (Si) with specific resistivity exceeding 10 kΩ·cm. FZ-Si substrates are indispensable for high-voltage power devices such as IGBTs and MOSFETs, which are widely used in applications including e-mobility, electric trains and power conversion (e.g. in renewable energy generation), and therefore are an important cornerstone for the energy transition. The purity and crystalline perfection of FZ-Si substrates ensure high efficiency, switching performance and lifetime of these devices.

The growth of crystals with larger diameter is a key objective for lowering costs in the production of semiconductor devices. Larger wafers enable a higher number of integrated circuits per wafer, thereby improving throughput and reducing the cost per device. However, scaling the crystal diameter in FZ-Si growth faces major technological challenges. At the Leibniz-Institut für Kristallzüchtung (IKZ), a dedicated research project in cooperation with PVA TePla focused on the growth of 200 mm FZ-Si crystals using a PVA-TePla FZ30-M furnace installed at IKZ. As part of these activities, crystals with diameter of up to 180 mm have already been achieved (see Fig.1). There are two main barriers limiting the scale-up of crystal diameter in the FZ process. First, thermomechanical stresses in the crystal increase with diameter, raising the risk of dislocation generation. The high radial temperature gradients appear because the latent heat generated at the crystallization interface scales with square of the diameter while the surface area for heat dissipation scales linearly. Second, the risk of electric discharge (arcing) at the high-frequency (HF) induction coil, which is the primary heat source in the process, increases with crystal size and required heat power. Addressing these challenges requires targeted development of FZ growth equipment, including optimized thermal shields and novel HF inductor designs. The HF inductor must provide an appropriate thermal field across all growth phases – from seeding, through cone growth, to steady-state cylindrical growth at full diameter.

Numerical modelling and machine learning were employed to guide equipment development. A numerical model of the FZ process implemented in COMSOL Multiphysics incorporated electromagnetic heating, heat transfer and phase boundary calculation for a given configuration. Model predictions showed that optimized inductor geometries and thermal shields can significantly reduce thermal stress and improve process stability for diameter enlargement. Machine learning techniques were used to correlate process parameters with growth stability metrics, enabling accelerated identification of optimal configurations [1].

A key quality parameter of FZ-Si wafers for power semiconductor applications is the radial resistivity variation (RRV). Low RRV across the Wafer is essential to ensure uniform device performance as variations in resistivity directly affect breakdown voltage and switching characteristics. The RRV is influenced by melt flow patterns during growth and segregation effects near the crystallization interface (diffusion boundary layer thickness), which depend on process parameters such as crystal rotation rate. In collaboration with the industry partner Siltronic AG, IKZ carried out a systematic study on the influence of key FZ process parameters on RRV and other crystal properties and process conditions such as the interface shape. Starting from a 4-inch reference process, more than 20 crystal growth runs were performed with controlled variations in crystal rotation and pulling rates. Lateral Photovoltage Scanning (LPS) was employed to determine the solid–liquid interface shape and four-point probe mapping was used for resistivity analysis. The data was used for validation and calibration of a numerical model of the FZ process developed by the project partner University of Latvia [2]. These results improved the predictive capability of the FZ process simulations for RRV control.

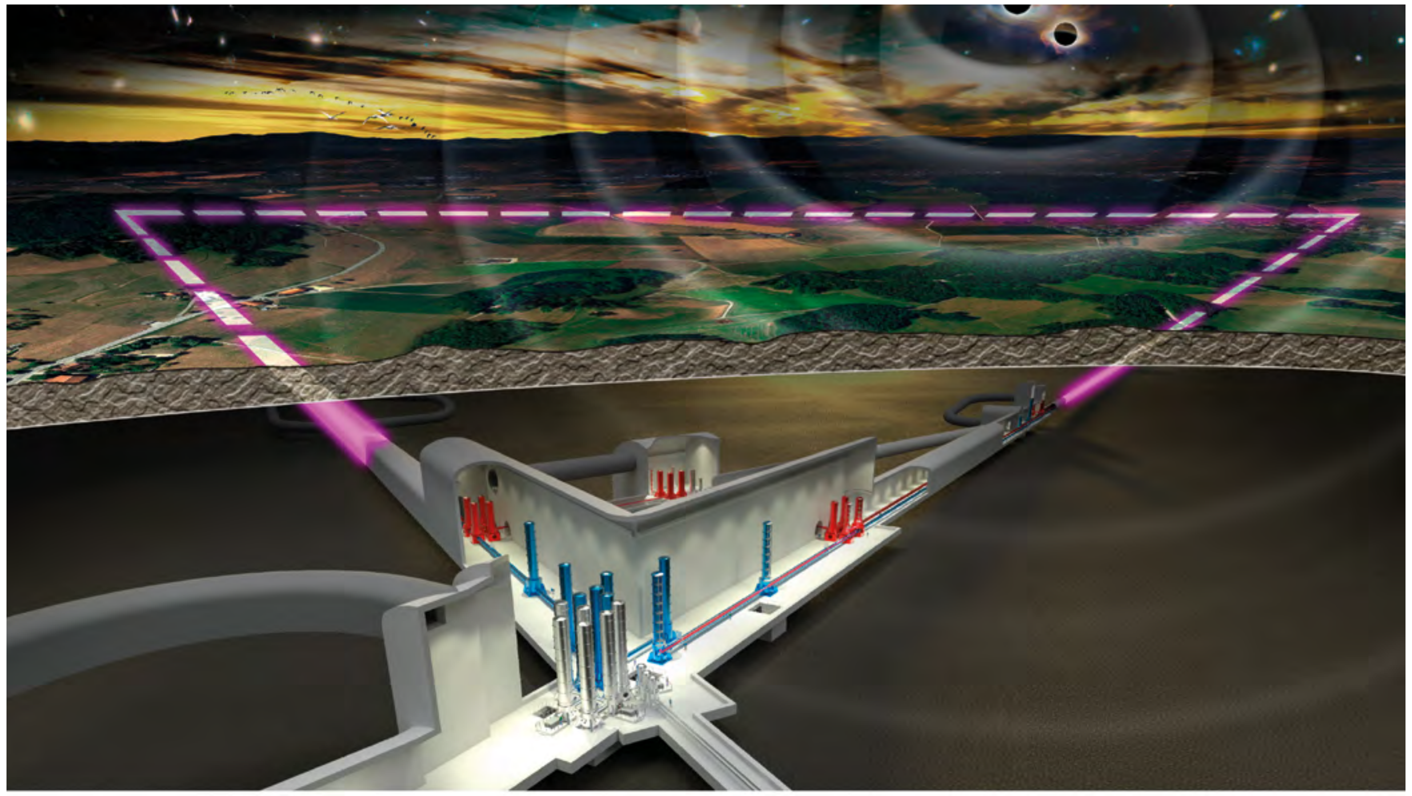


Fig. 2 Schematic illustration of the Einstein Telescope design *Photo: Marco Kraan/Nikhef*

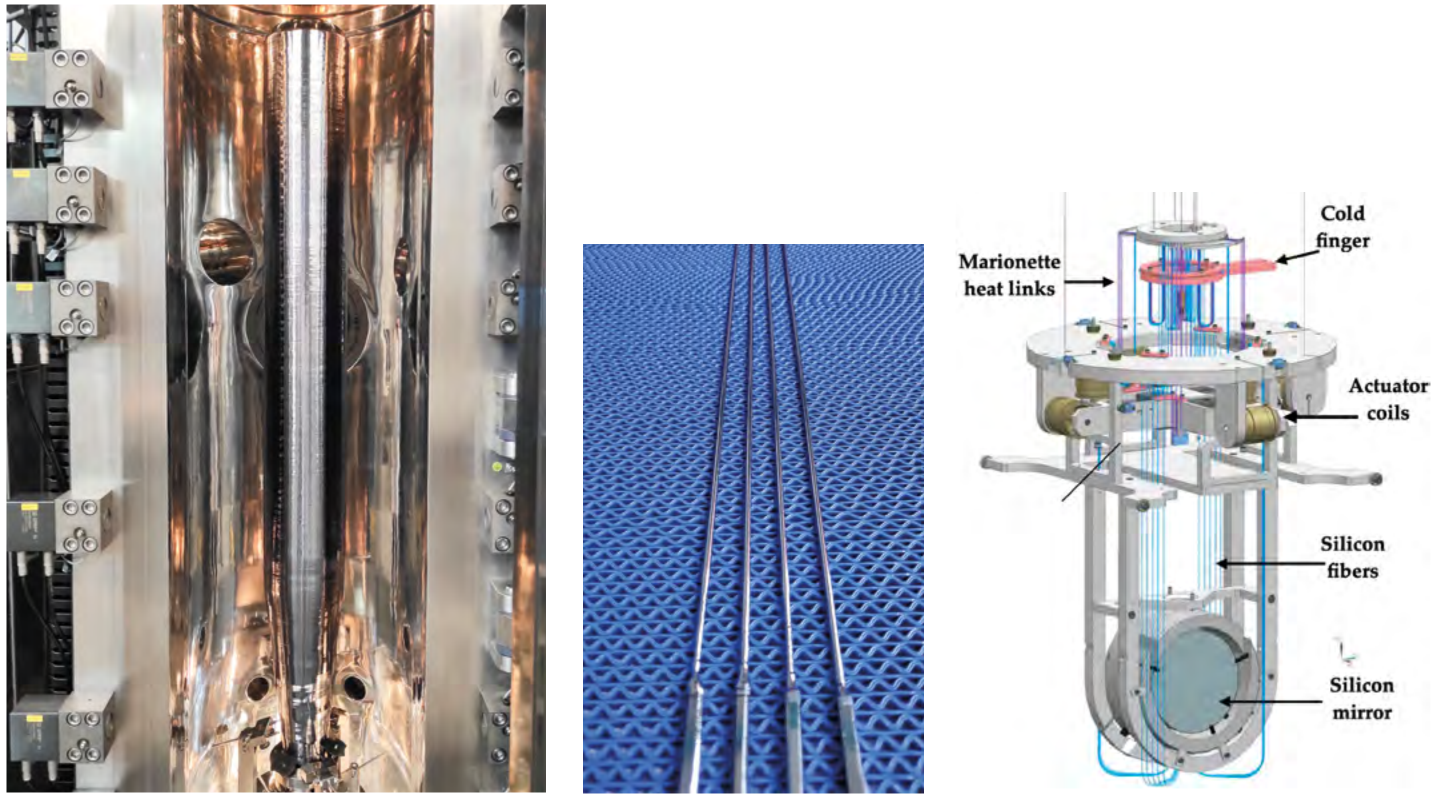


Fig. 3
Left: 6 inch FZ-Si crystal with ultrahigh purity, grown for ET mirror development at ET-Pathfinder *Photo: IKZ*
Middle: Si-Fibers for mirror suspension *Photo: IKZ*
Right: Mirror and mirror suspension at ETpathfinder *Source: Di Pace S. et al., Galaxies 10 (2022) 65*

FZ-Si for the Einstein Telescope

Third generation gravitational wave detectors such as the future Einstein Telescope (ET, see Fig. 2) will operate at cryogenic temperatures to minimize thermal noise and achieve unprecedented sensitivity. While current detectors such as Advanced LIGO and Virgo use fused silica mirrors at room temperature, silica becomes lossy when cooled and would strongly increase thermal noise. ET will overcome this limitation by using silicon mirrors cooled to around 20 K. Operating under these conditions will allow ET to observe more cosmic objects and look farther back in time than any other astronomical instrument.

The ideal material for the ET interferometer mirrors is silicon with ultrahigh purity and crystalline perfection. At cryogenic temperature, silicon exhibits a combination of unique material properties: it has a very low coefficient of thermal expansion near 20 K, very high thermal conductivity and a high mechanical quality factor. These properties ensure that thermal fluctuations of the mirror substrates are minimized, that residual heat from laser absorption can be efficiently extracted and that vibrational energy is stored with minimal loss.

The laser wavelength for the ET interferometer is projected to be around 1550 nm to enable the use of cryogenically cooled silicon mirrors. At this wavelength, absorption in silicon is dominated by residual impurities and free carriers. Float-zone (FZ) grown silicon, with its ultra-high resistivity (>10 kΩ·cm) and extremely low impurity content, achieves absorption coefficients below 5 ppm/cm. This outstandingly low absorption prevents excess heating of the cryogenic mirrors. Together with the very low mechanical loss of FZ-Si at low temperatures, it allows a substantial reduction of thermal noise and thereby directly enhances the sensitivity of the detector.

ETpathfinder, a prototype detector in Maastricht, is designed to test key technologies needed for the ET, with a focus on cryogenics and silicon test masses. Four large 6 inch high-purity FZ ingots with <100> orientation were grown at IKZ using the PVA-TePla FZ30 furnace and provided to ETpathfinder. The ingots were divided into sections to become test masses. One of those Ingots is shown in Fig. 3. Mechanical loss measurements showed no significant variations between the ingots, nor along the radial or longitudinal directions within each ingot. This consistency supports the high homogeneity and quality of the FZ material and demonstrates its suitability for cryogenic interferometer mirrors. For the ET much larger Si substrates are needed, with diameter of more than 450 mm. There are substantial barriers to achieving such crystal dimensions using the FZ method. As an alternative, the production of composite test masses from multiple FZ-Si substrates joined by direct bonding techniques is being investigated. This approach is a focus of ongoing research at the newly founded Deutsche Zentrum für Astrophysik (DZA) with IKZ as a partner.

The ET mirrors will be suspended by thin fibers, which must simultaneously isolate the mirrors from vibrations and extract heat generated by the laser beam. Silicon is an excellent material for this purpose because of its high thermal conductivity, high mechanical Q factor, and near-zero thermal expansion at cryogenic temperature. In the framework of a BMFTR funded project (No. 05A23BC1), IKZ has developed a dedicated growth setup for silicon fibers using the FZ technique. For this purpose, a Steremat FZ1505 furnace was modified to allow stable FZ growth of thin fibers with diameters in the millimeter range. The process development required precise control of the melt meniscus and optimization of growth parameters such as pulling rate and inductor shape. Fibers with a diameter of 3 mm and lengths exceeding 1 m were grown. The diameter uniformity along the fiber axis was better than ±0.1 mm (see Fig. 3). Optical inspection and X-ray topography confirmed that the fibers were free from dislocations and exhibited high crystalline perfection. Mechanical testing was carried out in collaboration with the University of Glasgow. The fibers showed a median breaking stress of 120 MPa, which is a promising value for application in suspension systems that must carry the expected load of the ET mirrors, which will reach more than 200 kg, while maintaining the required safety margins. These results represent an important step towards the fabrication of suspension fibers that meet the strict requirements of the ET. The next stages of the project will focus on tailoring the fiber geometry to allow reliable attachment to the test masses.

Further Information

einstein-teleskop.de

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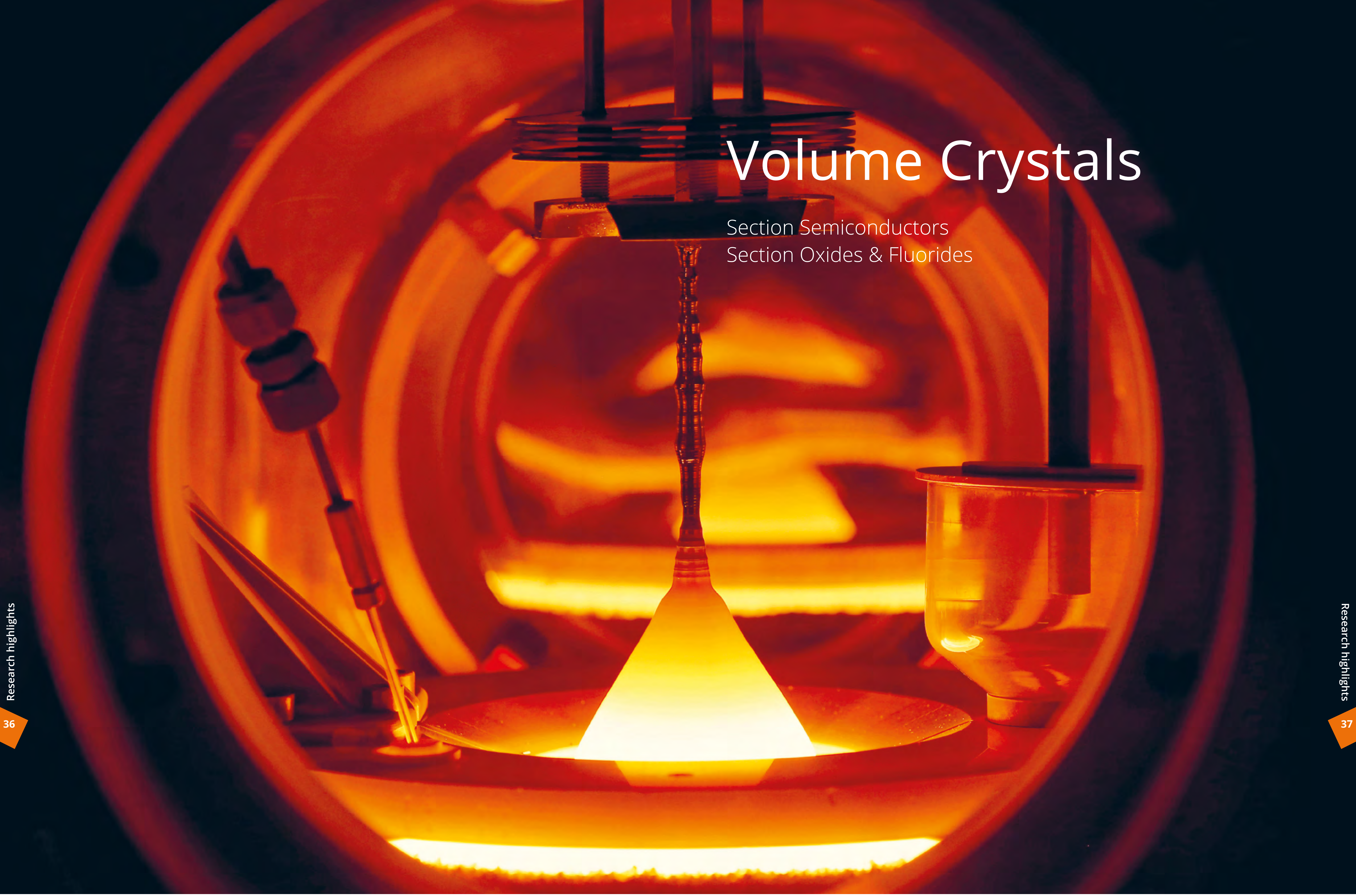

Volume Crystals

Section Semiconductors
Section Oxides & Fluorides

IKZ Annual Report 2024

Germanium single crystals *Photo: Simon Eichmann*

P. C. PALLETI, S. BERGMANN, U. JUDA, M. ALBRECHT, R. R. SUMATHI

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Purification and morphological analysis of high purity germanium

Germanium (Ge) is a vital material for next-generation electronics, infrared optics, optoelectronics, and microelectronics. In the field of radiation detection technologies, high-purity germanium (HPGe) is especially valued for its high energy resolution and sensitivity [1]. Applications such as nuclear safeguards, medical diagnostics, astrophysics, and environmental monitoring rely on HPGe detectors. For the efficient function of such detectors, Ge material must have extremely low impurity levels with net charge carrier concentrations below 10^{10} cm^{-3} (equivalent to 13N purity) and an engineered dislocation density within the range of 10^2 - 10^4 cm^{-2}, to enable full charge collection under reverse bias. Zone refining (ZR) process is the most effective method for producing ultra-high purity Ge [2], which offers better control, higher efficiency, and lower contamination risk. The technique involves melting a narrow region of the Ge metallic bar and moving it slowly along its length. As the molten zone moves, impurities redistribute between the solid and liquid phases based on the segregation coefficient k_0 (defined as C_S/C_L, where C_S and C_L are the concentrations in the solid and liquid). Impurities with $k_0 < 1$ (e.g., phosphorus (P), aluminium(Al)) tend to remain in the melt, whereas those with $k_0 > 1$ (e.g., boron (B), silicon (Si)) tend to move to the re-solidifying material. The efficiency of the ZR process and the yield of high-purity Ge are influenced by various factors such as container purity, ambient gas, and the process parameters like zone length and velocity. Among these, zone velocity is crucial, as it affects the effective impurity segregation (k_{eff}) as well as the diffusion.

In this study, we examined the effect of various ZR velocities on the purification efficiency. As a starting material, a Ge metal bar with a net carrier concentration of around 5 - 9 × 10^{11} cm^{-3} with a *p*-type conductivity was used. Multiple ZR with a low velocity of 1 mm/min (in a quartz container coated with quartz-smoke (SiO_2) layer) led to increased carrier concentration (~ 3 × 10^{12} cm^{-3}) and further changed the conductivity type (to *n*-type). This contamination was likely due to prolonged contact between the melt and the coating, which enhanced the diffusion of impurities from the SiO_2 into the Ge melt. In addition, oxygen from the quartz container/coating might form inactive complexes with Al and prevent its removal. In contrast, refining at a moderate speed of 4 - 5 mm/min produced better results, with carrier concentrations between 10^{11} - 10^{12} cm^{-3} maintaining *p*-type conductivity [2].

Based on these insights, optimum zone velocity was utilised further, and a two-stage ZR process was developed to produce 13N-purity Ge. In the first stage, 4N Ge was purified in a graphite container under N_2 gas (Fig. 1a). This step effectively segregated Al, resulting in *p*-type Ge bars (Fig. 1c) with net carrier concentration of around 2 × 10^{12} cm^{-3}. The impure ends were cropped, and the remaining bar underwent the second stage, where ZR was performed in a coated quartz container under H_2 ambient (Fig. 1b). This process is repeated again, and the finally obtained HPGe bars (Fig. 1d) have a net concentrations in the range of 4 - 9 × 10^{10} cm^{-3}, demonstrating the optimization of the ZR process.

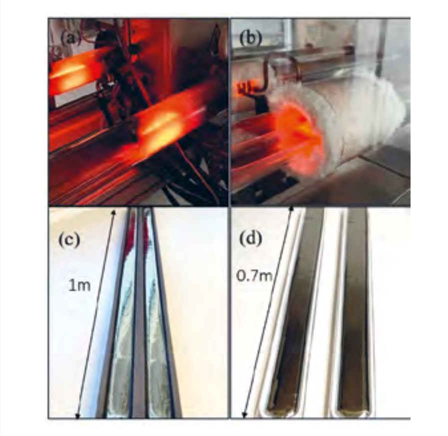

Fig. 1 (a) Initial zone refining process carried out in in graphite containers at N_2 atmosphere; (b) the final ZR process carried out in quartz containers at H_2 atmosphere; (c) one meter long (approx. 5 - 6 kg) of 10N pure Ge-bar within a graphite container, (d) final ZR Ge bars of 13 N purity with 70 cm length. From [2] under license CC BY 4.0.

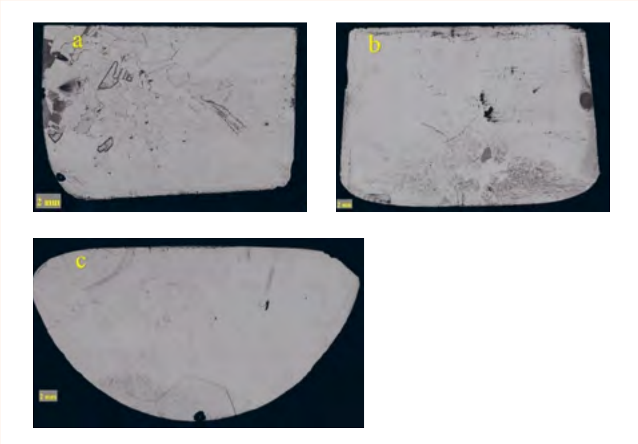

Fig. 2 The microstructures of wafers prepared from ZR polycrystalline Ge, refined in different gas atmosphere: (a) argon; (b) nitrogen; (c) hydrogen. From [2] under license CC BY 4.0.

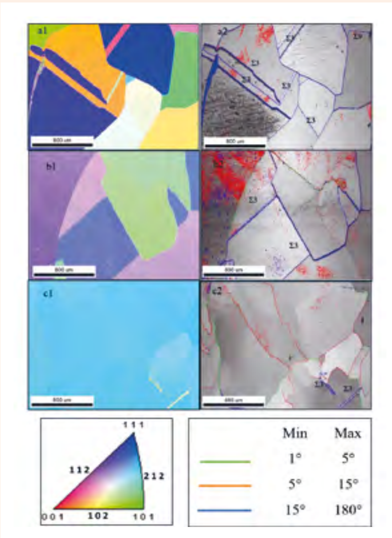

Fig. 3 EBSD analysis of the Ge, zone refined in different ambient gases (a) argon; (b) nitrogen; (c) hydrogen. From [2] under license CC BY 4.0.

To better understand the material quality, morphological analysis was carried out on polycrystalline Ge refined under different gas atmospheres. Optical microscopy analyses (Fig. 2) following the wet-chemical etching revealed grain boundaries (GBs), and distinct differences in dislocation structures with ZR conditions. Ge refined in a graphite container under argon shows multiple small grains and high dislocation density. Under nitrogen, larger grains formed at the top, with dislocation clusters at the bottom. Ge refined under hydrogen in a quartz container exhibited larger grains and minimal number of dislocations. Electron backscattering diffraction (EBSD) analyses confirmed these trends: Ge zone refined in argon and nitrogen shows high-angle grain boundaries (HAGBs) such as Σ3 and Σ9, while ZR under hydrogen primarily showed low-angle GBs (LAGBs) in Ge, as shown in Fig. 3. The grain size and the formation of HAGBs/LAGBs further depend on various conditions such as cooling rate, thermal gradient, container material, and initial impurity content in Ge source, and influencing growth kinetics [2].

Charge carrier lifetime (τ), measured on different samples by microwave-detected photoconductivity decay, exhibited the highest minority carrier lifetime (~50 µs) for the Ge refined under hydrogen as compared to 10-35 µs for argon and nitrogen. Reduced lifetimes for argon and nitrogen cases is due to dislocation clusters, HAGBs, and residual impurities acting as recombination centres. These results highlight that the zone refining process is very efficient under hydrogen atmosphere.

Acknowledgements

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LiNbO$_3$ crystal *Photo: Moritz Thau*

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Phase diagram of the system LiNbO$_3$—LiTaO$_3$

The DFG research unit FOR5044 is focused on systematic investigations of polar oxide lithium niobate-lithium tantalate (LiNb$_{1-x}$Ta$_x$O$_3$, LNT) solid solutions. Due to the miscibility over the entire compositional range as well as the tunable ferroelectric domain structure, these crystals represent a model system for uncovering and application of novel phenomena in material science and physics. The exceptional thermal stability of the system, as well as the inherent point defects, domain structure, and their interaction open up a novel and broad range of emerging applications not only in high-temperature sensor and actuator technologies, but also in integrated acoustics and photonics. Examples include piezoelectric sensors that operate at elevated temperatures under harsh environments thereby contributing to efficient energy conversion and components for the domain wall electronics and optoelectronics. IKZ is part of the research unit and creates the materials basis for the experimental work of all other projects contributing to the goals of the entire unit. In particular, we focus on the study of the melting phase diagram LiNbO$_3$—LiTaO$_3$, of fundamental thermophysical properties of LNT solid solutions, and last but not least on the provision of tailored samples to project partners.

For the successful design of an appropriate crystal growth process, solid knowledge of the respective materials system by means of a melting phase diagram is essential. For LNT solid solutions this refers to the system LiNbO$_3$—LiTaO$_3$ that was studied in not great detail in the early years of the 'oxide research' [1]. Yet this study allowed for the important conclusion that both end-members most likely form solid solutions without any gap. However, comparing our own findings and those of others [2] with Peterson's results it becomes clear that the component segregation observed in the crystal growth experiments seems to be much lower than in the proposed phase diagram. Here one could argue that in the crystal growth an effective segregation coefficient comes into play. But taking into account the rather low applied pulling rates, the commonly excepted Burton-Prim-Slichter model results in a negligible deviation of the effective segregation coefficient from the equilibrium one that can be read from the phase diagram. This discrepancy prompted us to analyse the phase diagram in more detail [3].

As a first approximation we assumed that both, the liquid and the solid phase behave ideally, that is the total Gibbs free energy of both can be computed from the weighted average of the Gibbs free energies of the end-members plus a contribution related to mixing. Under this presumption, only very few data is needed, i.e. the melting point temperatures and the corresponding heats of fusion of both end-members that can be easily measured, to calculate the liquidus and solidus curves using the Schröder-van Laar equation [4]. The resulting phase diagram is a surprisingly good match to Peterson's diagram but deviates significantly from the findings of the crystal growth experiments. From that we conclude that there must be substantial non-ideal ('excess') contributions to the Gibbs free energy of the system and that a thorough thermal analysis of the system is required.

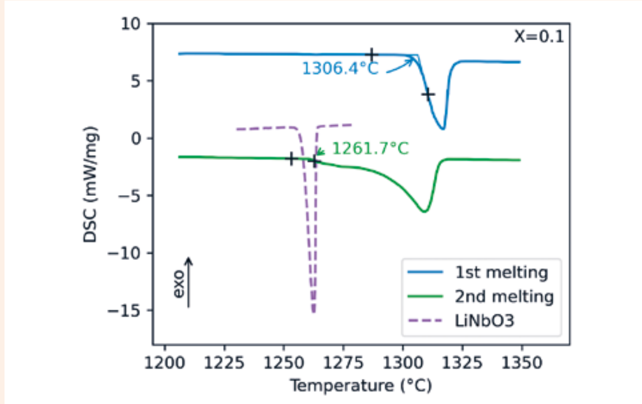

Fig. 1 Melting behaviour of LNT solid solutions: Compared with pure LiNbO$_3$ (dashed pink curve) the melting peak is much broader for solid solutions, here Li(Nb$_{0.9}$Ta$_{0.1}$)O$_3$. As a result of segregation during solidification, broadening is enhanced upon second melting of the sample (green curve) and the onset is shifted towards the melting temperature of pure LiNbO$_3$.

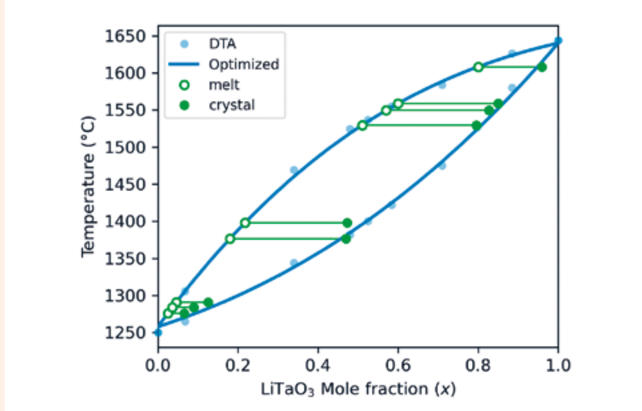

Fig. 2 Optimized version of the LiNbO$_3$—LiTaO$_3$ phase diagram based on our DTA investigations considering non-ideal behaviour of the solid phase. Crystal growth experiments are represented by pairs of compositions corresponding to the initial material input (liquid composition, empty circles) and crystal output (solid composition) connected by horizontal lines. The ordinate of these pairs was chosen so that the point corresponding to the liquid composition lies on the liquidus curve.

A series of LNT solid solution compositions were characterized by differential thermal analysis (DTA). Here, the sample is heated to a temperature above the melting temperature and compared to a reference sample with way higher melting temperature. Whenever the sample undergoes a phase transition, a certain amount of heat is consumed (endothermic process, e.g. melting) or released (exothermic process, e.g. crystallization), and a temperature difference between the sample and the reference is observed. Fig. 1 shows such melting curves for an LNT solid solution along with that of pure LiNbO$_3$. It can be seen that compared with the pure compound, the melting peak of a solid solution is less 'intense' and stretched over a wider temperature range. In subsequent heating cycles this stretching becomes stronger and the thermal effect becomes more and more blurred. We interpret the onset temperatures during the first melting cycle as solidus temperatures and the temperature at which the DTA curve returns to the baseline after the melting as liquidus temperatures in the phase diagram.

In result we obtained a set of solidus and liquidus temperatures for various solid solution compositions. In the next step we used these and Gibbs free energy data of the end-members as input for the phase diagram optimization. In the optimization the liquid phase is treated as an ideal mixture. For the solid phase, however, non-ideality is considered by means of an excess contribution to the Gibbs free energy. This excess energy is expressed as a series of Redlich-Kister polynomials the parameters of which are varied during the optimization routine.

The optimized phase diagram (Fig. 2) is in excellent agreement with the crystal growth experiments. It allows for a better design of the crystal growth process including adjustment of melt composition with respect to a required crystal composition, tuning of growth parameters to ensure a desired chemical homogeneity and process stability. This assessment forms the basis for the ongoing study of doping and stoichiometry control in the LiNbO$_3$—LiTaO$_3$ solid-solution system. This is the main research topic of our group during the second part of FOR5044, for which funding was recently acquired until 2029.

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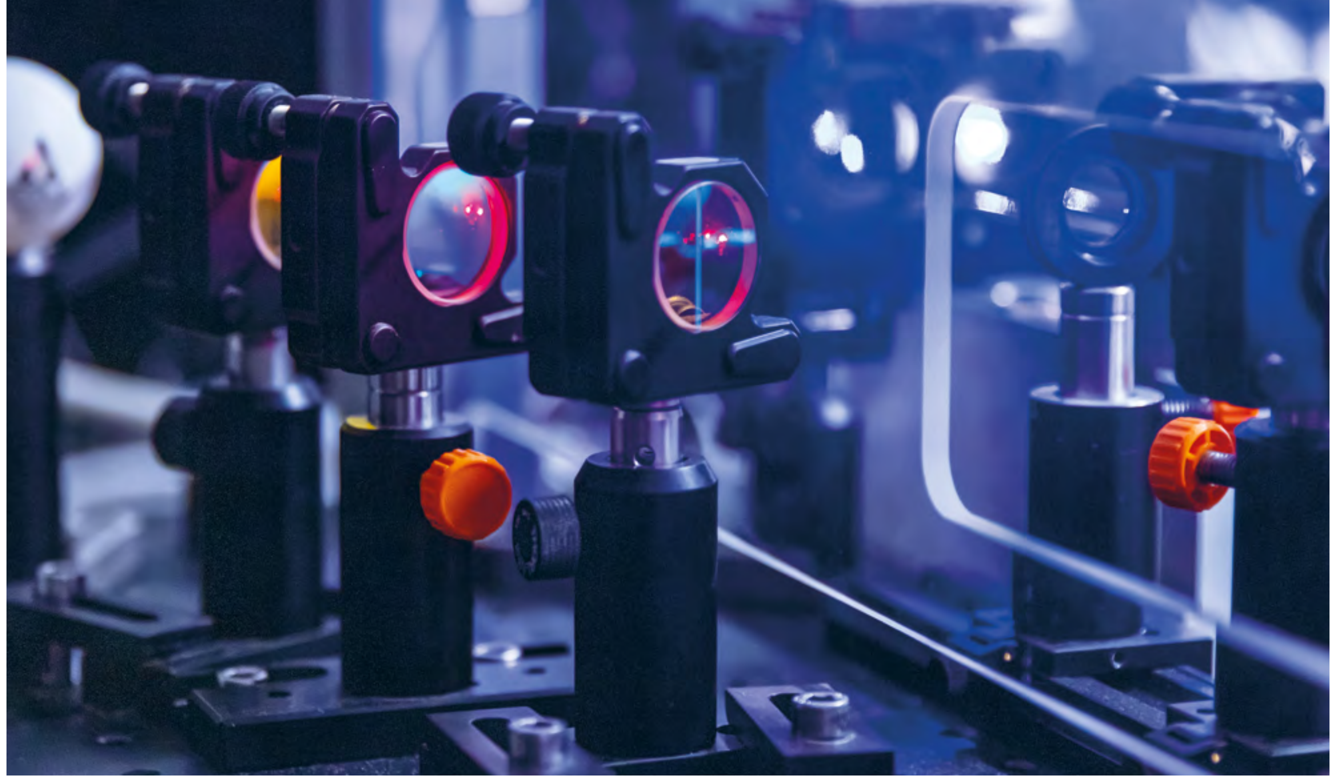
Research highlights



Visibly emitting Pr:YLF laser *Photo: Berit Kraushaar*

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Growth of $BaMgF_4$ for continuous-wave frequency conversion to vacuum UV

Coherent light sources in the ultraviolet (UV) spectral range are of significant importance across various fields of research and industry. Traditionally, these light sources have been realized through successive nonlinear frequency conversion of powerful near-infrared lasers using well-established nonlinear oxide crystals. Recently, the development of a nuclear clock based on thorium-229 (Th-229) has triggered a new demand for narrow-line coherent light sources at wavelengths around 148 nm [1]. Th-229, an artificial radioactive isotope, possesses a nuclear excited state with an exceptionally low excitation energy—referred to as an isomer—making it accessible with laser technologies. Unlike electronic transitions used in conventional atomic clocks, nuclear transitions are far less sensitive to external electromagnetic fields, promising unprecedented clock stability and accuracy. This unique property could enable Paul-trap-free, all-solid-state nuclear clocks using Th-229 embedded in UV-transparent crystals such as CaF_2. However, the realization of the Th-229 nuclear clock critically depends on the availability of narrow-line CW light sources at ~148 nm, a requirement for which no existing technology is currently sufficient. This limitation stems mainly from the absence of suitable nonlinear optical crystals that are transparent at such short wavelengths.

Nonlinear frequency conversion based on noncentrosymmetric fluoride crystals is considered a promising pathway. Fluoride materials possess wide bandgaps, offering transparency down to approximately 120 nm. However, they exhibit second-order nonlinear optical coefficients $\chi(2)$ that are orders of magnitude smaller than those of traditional nonlinear crystals. Furthermore, since birefringent phase matching is not feasible in fluoride crystals owing to their relatively small birefringence, the material must be ferroelectric to enable quasi-phase matching (QPM) through periodic poling.

Barium magnesium fluoride ($BaMgF_4$, BMF) is a highly promising candidate for nonlinear frequency conversion into the vacuum-ultraviolet (VUV) spectral region. BMF is an orthorhombic, polar-structure crystal belonging to the point group mm2, offering ferroelectricity with a reasonably small coercive field required for ferroelectric domain switching. In 2024, IKZ and Fraunhofer IPM teamed up and started a collaborative project UV-KrisP, to develop the key technologies necessary for realizing periodically poled BMF crystals for VUV applications. This project is funded by the German Federal Ministry of Research, Technology and Space under the Quantum Systems research program. Within this collaboration, IKZ is responsible for growing high-quality BMF single crystals, while Fraunhofer IPM focuses on developing techniques for achieving sub-nanometer periodic poling of BMF through ferroelectric domain engineering. Together, these efforts aim to pave the way toward the first VUV-capable nonlinear optical converter based on periodically poled fluoride crystals.

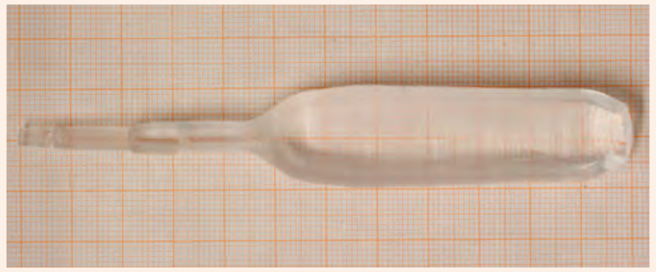

Fig. 1 Photograph of a Czochralski-grown BMF single crystal.

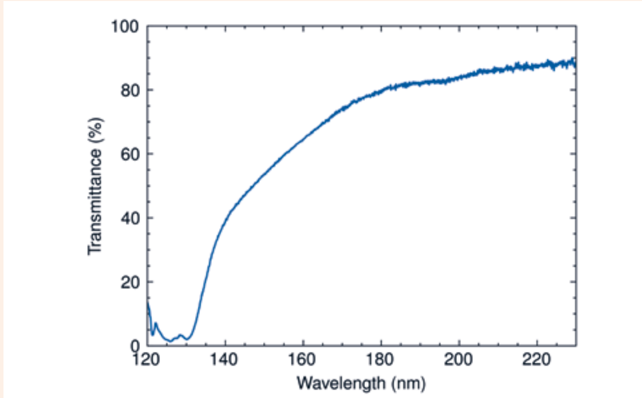

Fig. 2 VUV transmission spectrum of an 8-mm-long BMF crystal.

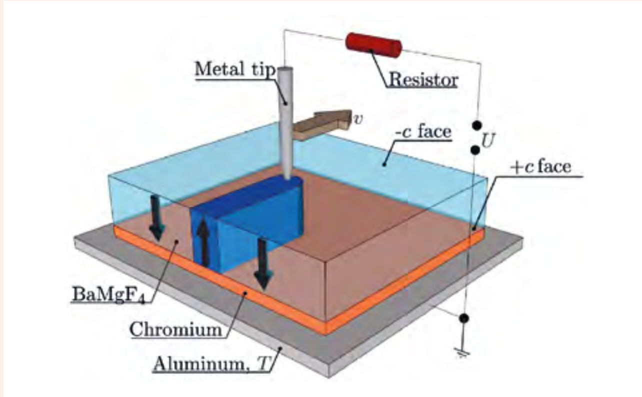

Fig. 3 Illustration of calligraphic poling setup at Fraunhofer IPM [2].

Figure 1 presents one of the latest $BaMgF_4$ (BMF) single crystals grown using the Czochralski technique. Achieving high transparency in the VUV spectral range (below 200 nm) critically depends on minimizing water contamination during the crystal growth process. The presence of hydroxyl (OH) impurities, introduced by water, severely degrades the UV transparency of the crystal. Leveraging extensive expertise and decades of experience in fluoride single crystal growth at IKZ, we have successfully grown BMF crystals with exceptional VUV transparency. Figure 2 shows the transmission spectrum of an 8-mm-long BMF crystal, measured using a VUV transmission spectrometer. The crystal exhibits no detectable OH impurity absorption and achieves an internal transmittance exceeding 50% at 150 nm-representing the highest UV transparency ever reported for BMF crystals to date.

Our partner, Fraunhofer IPM, has successfully demonstrated smooth periodic poling of BMF crystals using the calligraphic poling technique. This method enables direct writing of ferroelectric domains by controlling the trajectory of a moving metal tip, which acts as the top electrode, while a thin chromium layer sputtered onto the surface of a 0.5-mm-thick (001)-oriented polished wafer serves as the planar bottom electrode. Figure 3 illustrates the setup used for calligraphic poling. To investigate the angle-dependent domain switching behavior of BMF, radially oriented domains were written, revealing the material's poling anisotropy. A fanout periodic poling pattern spanning an angular spectrum of approximately 14° was successfully demonstrated. More details on the crystal growth and periodic poling can be found in [2].

Although our BMF crystals exhibit the highest UV transparency reported to date, there is scope for further improvement. This will be pursued through continued optimization of growth parameters, guided by a deeper understanding of BMF crystallization behavior. We are at the forefront of developing VUV coherent light converters based on BMF, and within the scope of this project, we aim to demonstrate efficient frequency conversion into wavelengths below 200 nm.

Acknowledgements
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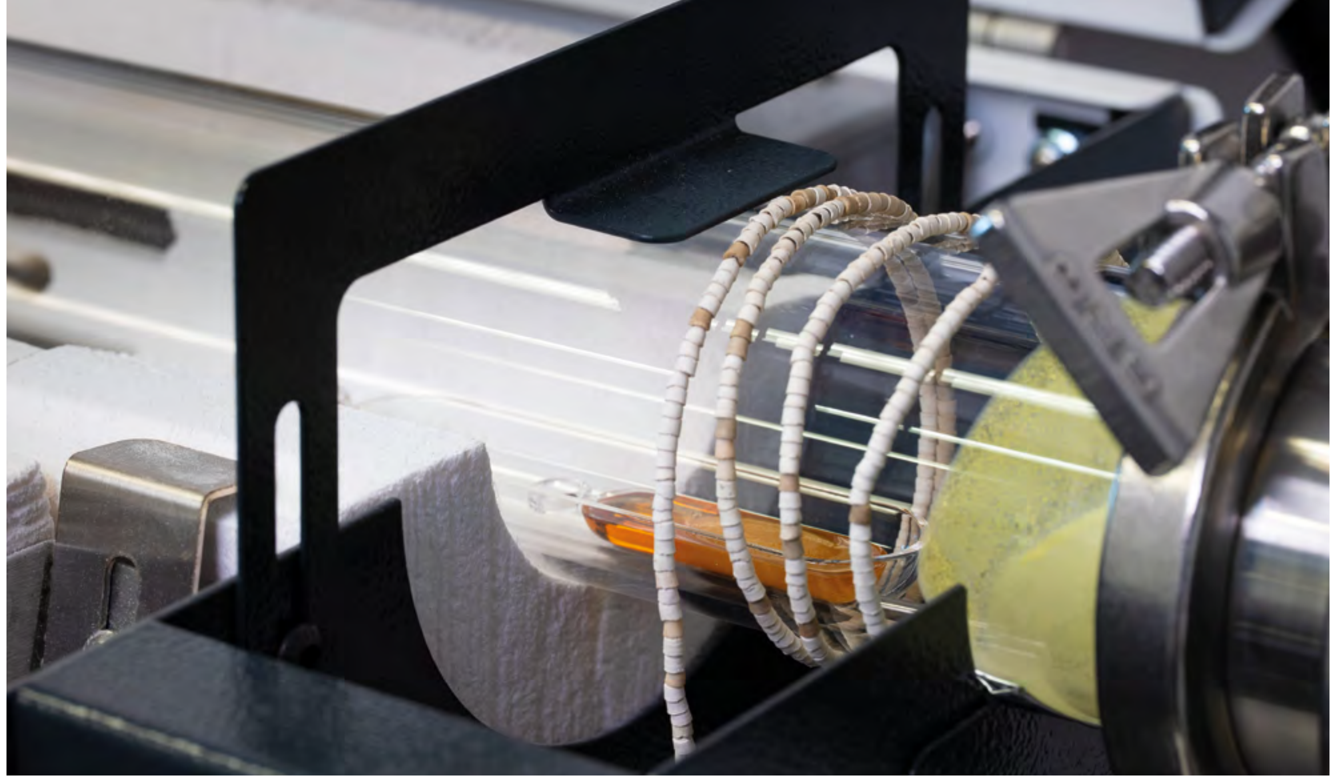
Nanostructures & Layers

Section Semiconductor Nanostructures
Section Thin Oxide Films



Detail of chemical vapour deposition (CVD) furnace: Quarz tube, Sulphur-crucible and local heating wire *Photo: HORNNISSEN*

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Y-Stabilized ZrO_2 as promising substrate for the epitaxial growth of transition metal dichalcogenides

Two-dimensional (2D) semiconductors, in particular transition metal dichalcogenides (TMDCs) such as MoS_2, have attracted considerable interest as they promise to extend Moore's Law beyond silicon and are considered next-generation optoelectronic materials. To fully explore the potential of 2D-TMDCs, single-crystalline wafer-scale films with tuneable material composition, layer thickness, and high crystalline quality are needed. However, the synthesis of 2D-TMDCs that meet these requirements constitutes a major obstacle towards technological integration. Although wafer-scale epitaxial growth of graphene and hexagonal boron nitride has been reported, these techniques are not applicable to the growth of TMDCs due to different growth kinetics. Hence, the direct growth of wafer-scale single-crystalline TMDCs on insulating substrates remains challenging. The selection of suitable substrates is limited not only by purely crystallographic considerations, but also by the resistance of the wafer to melting, decomposition, and chemical reactions with chalcogen atoms at elevated temperatures.

Sapphire is commonly used as substrate for epitaxial growth. However, the in-plane lattice mismatch between classical TMDCs (e.g. 2H-polytype MoS_2 a_{MoS2} = 3.161 Å) and sapphire (a_{Al2O3} = 4.76 Å) is more than 30%. Due to coincidental matching of multiple lattice units, two types of in-plane rotational domains have been reported: The first configuration corresponds to the 3 x a_{TMDC} ≈ 2 x a_{Al2O3} supercell. The second variant involves a 30° rotation of the TMDC lattice with respect to sapphire yielding a larger supercell consisting of five TMDC units (5 x a_{TMDC} ≈ 2 √(3) x a_{Al2O3}, R30° configuration). Although the R30° configuration is expected to be energetically favourable, both variants are observed and there are only very few reports on single-crystalline wafer-scale growth [1, 2]. Apparently, it is difficult to control all relevant growth parameters motivating the search for alternative substrates providing more stable epitaxial growth conditions.

We have shown that cubic yttrium-stabilized zirconium dioxide (YSZ) could be an alternative to sapphire and replace it as a widely available substrate for TMDC growth [3]. Specifically, we demonstrated epitaxial growth of MoS_2 on YSZ with pure six-fold symmetry for both physical- (PVD) and chemical vapor deposition (CVD) processes. Zirconium dioxide ZrO_2 is generally known as a substrate for In_2O_3-based bixbyite compounds and can be stabilized by yttrium (Y) as a face-centred-cubic fluorite structure with a lattice parameter which depends on the Y-molar fraction. With a nominal Y doping level of 9 mol%, the in-plane lattice spacing along the [1-10] direction is $a_{YSZ\ 1\text{-}10}$ = 3.639 Å. This coincides much better with the in-plane lattice parameter of 2H-MoS_2 reducing the lattice mismatch to –13%.

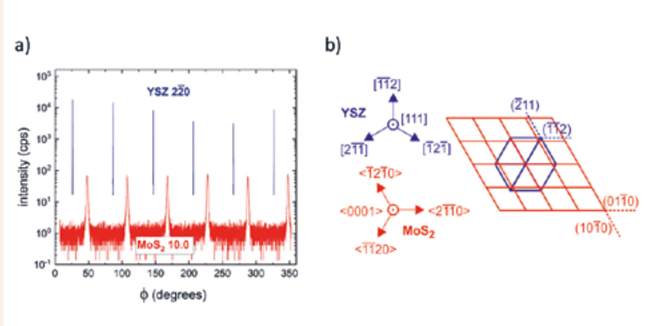

Fig. 1 a) GIXD in-plane X-ray diffraction rocking curves (ϕ-scans) of the YSZ wafer (blue) and the MoS_2 layer (red), taken at 2θ = 32.9° (MoS_2 10.0 Bragg reflection) and at 2θ = 49.7° (YSZ 2-20 Bragg reflection). b) Epitaxial relationship scheme of YSZ wafer (marked in blue colour) and MoS_2 layer (marked in red colour).

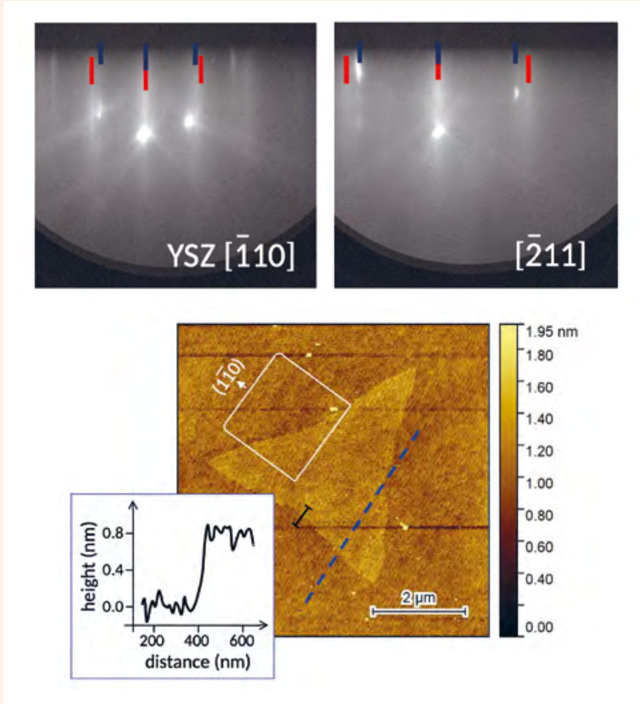

Fig. 2 MoS_2 layer grown by CVD on YSZ (111) substrate. a) RHEED patterns of the sample recorded along the [-110] and [-211] directions of the YSZ wafer. Bragg reflections of the YSZ wafer and MoS_2 are highlighted by the red and blue lines, correspondingly. b) Overview AFM image of the triangular domain and the height profile along the black line. The blue line depicts the direction of atomic step edges of the wafer.

First, we address the PVD growth of multilayer and monolayer (ML) films. In-plane x-ray diffraction under grazing incidence (GIXD) was performed to determine the full epitaxial relationship between the MoS_2 layer and the YSZ substrate. Figure 1a shows two in-plane rocking curves (ϕ-scans) taken at 2θ = 32.9° (corresponding to the MoS_2 10.0 Bragg reflection) and at 2θ = 49.7° (corresponding to the YSZ 2-20 Bragg reflection), both exhibiting six-fold in-plane symmetry. The width $\Delta\phi_{sub}$ = 0.1° of the substrate reflections matches approximately the experimental angular resolution, while the layer reflections are noticeably wider ($\Delta\phi_{layer}$ = 1.8°). However, the in-plane mosaic spread is more than a factor of 2 smaller than for MoS_2 layers grown on sapphire. From the relative position of layer and substrate reflections, it is evident that the MoS_2 {10-10} net-planes are oriented parallel to the YSZ (-211) net-planes (see Figure 1b). No other Bragg reflections attributable to the MoS_2 layer appear. The in-plane lattice parameter a_{exp} = 3.14 Å derived from 2θ/ϕ- scans, is very close to the literature value for bulk MoS_2, indicating a fully relaxed layer.

To further prove the suitability of YSZ for epitaxial growth of TMDCs, we performed also CVD growth experiments. The layer orientation verified by ex-situ reflection high energy diffraction (RHEED) coincides with that found in the PVD samples (Figure 2a). A closer inspection by AFM reveals that one of the zigzag edges of the MoS_2 triangle is aligned perpendicular to the atomic steps of the substrate with a miscut of 0.2° toward the [1-10] direction (Figure 2b). Statistical analysis of MoS_2 triangles reveals that this alignment holds for 93% of the domains. The minor variant corresponds to a 30° rotation of the MoS_2 crystals.

The observed domain nucleation and growth process provides excellent perquisites for the fabrication of single-oriented TMDC layers on the YSZ substrate. Careful design of the wafer miscut orientation will play an important role in the further development of a single crystalline growth process.

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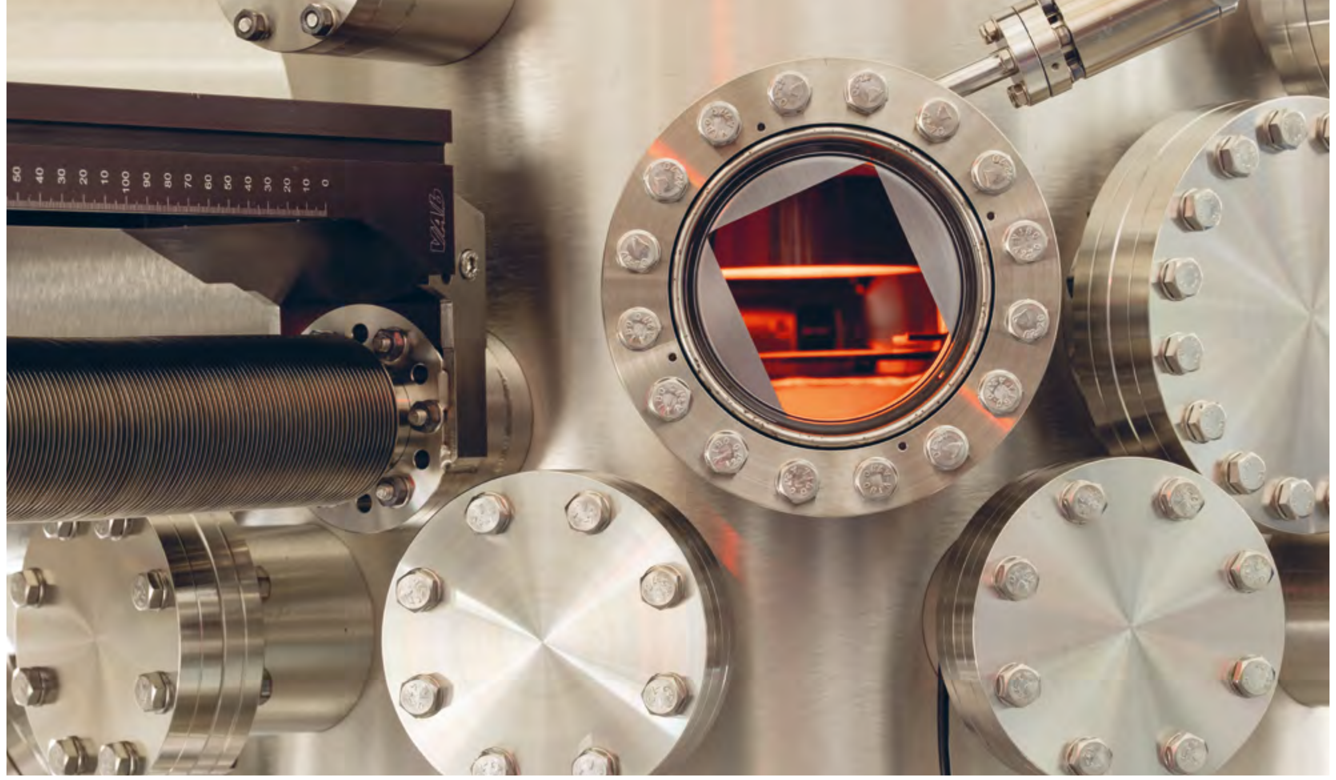

Molecular beam epitaxy chamber for isotope-pure SiGe quantum materials *Photo: HORNNISSEN*

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Advances in SiGe epitaxy and surface characteriztion using atomic force microscopy and Raman spectroscopy

Silicon-germanium (SiGe) epitaxy plays a key role across a wide range of advanced technologies in microelectronics, optoelectronics, and, increasingly, in quantum technologies. Recent interest in SiGe has grown significantly due to its potential for enabling spin qubits in isotopically purified, nuclear spin-free materials, which are essential components in scalable quantum computing.

At IKZ, research efforts focus on preparing epi-ready SiGe substrates and growing defect-free isotopically purified epitaxial films on reversed-graded SiGe virtual substrates. These heterostructures are integral to the realization of gate-defined silicon quantum dots, a fast-evolving platform for quantum technologies.

Pit-formation in Ge homoepitaxial layers

A critical aspect of achieving high-quality epitaxial films is the control of surface contamination and defect formation. Our investigations into germanium homoepitaxy have highlighted the impact of residual carbon and oxygen – introduced during conventional wet chemical cleaning – on the formation of macroscopic growth defects, such as pits [1]. These defects arise due to the strong affinity of carbon to the Ge surface, where it tends to cluster and nucleate undesirable features.

Pit densities ranging from 10^6 to 10^9 cm^{-2} were observed, with their formation closely tied to the epitaxial growth conditions. Within the ideal growth temperatures for flat Ge layer epitaxy, the pit density decreases in the range from 300°C to 400°C but remains non-zero.

Atomic force microscopy (AFM) provided detailed insights into the three-dimensional topography of these pits as shown in Fig. 1a and 1b, revealing dominant crystallographic facets such as {113} and {3 15 23}, both known to appear in epitaxial Ge surfaces.

To mitigate pit formation completely, we developed a refined process involving a high growth-rate room-temperature buffer layer growth (0.02 nm/s). This approach effectively encapsulates residual contamination and promotes a fresh, defect-free surface for subsequent epitaxy. These advances are particularly relevant for the fabrication of isotopically pure Ge layers, currently under further investigation in collaboration with our quantum research partners.

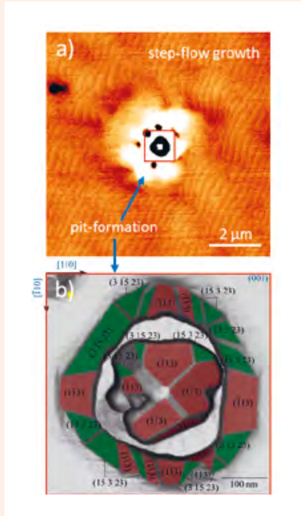

Fig. 1 a) AFM image presenting the morphology of as-grown surface of Ge homoepitaxial layer exhibiting step-flow growth and formation of a macroscopic pit defect. b) shows plane view 3D figure of the pronounced pit with indexed facet planes mostly of {113} and {15 3 23}. Reprinted from [1] according to CC BY 4.0 license.

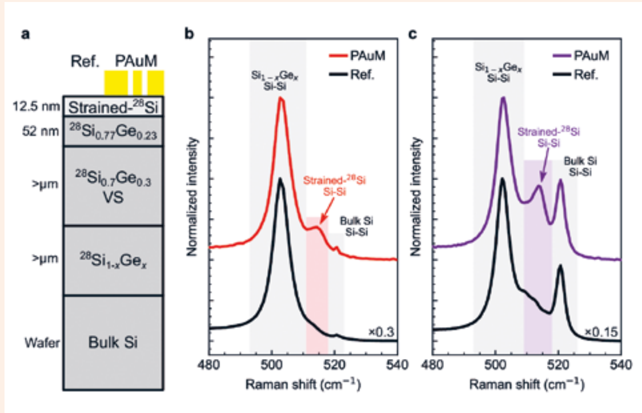

Fig. 2 a) Sketch of the strained ^{28}Si thin film and its substrate. The compound is partially covered by a PAuM. Raman spectra of the strained ^{28}Si thin film with PAuM (red line in b and purple line in c) and without PAuM (black lines), collected using a 638 nm (b) and a 785 nm (c) laser. Reprinted from [2] according to CC BY 4.0 license.

Probing strain in Si/SiGe quantum wells via surface-sensitive Raman spectroscopy

In gate-controlled spin qubit architectures, uniform strain across Si/SiGe quantum wells is crucial, as strain directly affects the energy landscape experienced by qubit arrays. However, due to the ultrathin nature of these layers (~10 nm), conventional strain characterization poses significant challenges.

To address this, a novel surface-sensitive Raman spectroscopy technique utilizing porous gold membranes (PAuM) was developed and employed in an collaborative effort spearheaded by the group of Sebastian Heeg at Humboldt-Universität zu Berlin. This method enables rapid, spatially resolved mapping of micrometer-scale strain fluctuations, such as those appearing in the characteristic cross-hatch patterns of strained SiGe layers, without the need for ultraviolet (UV) Raman setups.

In a representative structure, a thin strained ^{28}Si layer was grown via molecular beam epitaxy (MBE) on a relaxed $^{28}Si_{0.7}{}^{76}Ge^{0.3}$ virtual substrate, as shown in Fig. 2. Applying a PAuM directly to the sample enhanced surface sensitivity, allowed Raman signals to be extracted specifically from the ultrathin top layer. Comparative spectra obtained using 638 nm and 785 nm excitation (Fig. 2b and c) showed surface-to-bulk signal suppression factors of 3.5 and 6.5, respectively, confirming the effectiveness of the PAuM-enhanced Raman technique.

The observed phonon softening in the strained Si peak indicated tensile strain, and quantitative analysis yielded an average strain of 0.95% ± 0.02%. This result aligns closely with values derived from high-resolution X-ray reflectometry (1.0%) and, critically, opens new avenues for high-resolution strain mapping, central to our ongoing collaborative work.

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Liquid-delivery spin MOVPE reactor for the epitaxy of ferroelectric (K,Na)NbO_3 thin films *Photo: Matthias Kern*

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Determination of the optical constants of epitaxial $K_{0.85}Na_{0.15}NbO_3$ thin films in the monoclinic and orthorhombic phase

Ferroelectric oxide materials are used in a wide range of optical applications as e.g. sensors, electro-optic modulators or infrared detectors. These materials are characterized by nonlinear optical properties, high transparency and large index of refraction in the visible spectral range. Potassium-sodium-niobate (K,Na)NbO_3 is a lead-free ferroelectric perovskite with attractive optical properties mentioned above. (K,Na)NbO_3 thin films grown under anisotropic compressive lattice strain exhibit a monoclinic symmetry at room temperature (M_c-phase) and an orthorhombic symmetry at higher temperatures (c-phase) [1] making it an ideal system for studying the influence of the phase symmetry on the dielectric properties. In the present work, we apply spectroscopic ellipsometry (SE) to determine the optical constants in the spectral range of 0.7 – 6 eV of a ferroelectric $K_{0.85}Na_{0.15}NbO_3$ thin film both for the monoclinic M_c-phase and the orthorhombic c-phase. These results are published in Ref. [2].

$K_{0.85}Na_{0.15}NbO_3$ thin films were grown on IKZ-own (110) $Gd_{0.6}Sm_{0.4}ScO_3$ substrates by liquid-delivery spin metal-organic vapor phase epitaxy. From temperature dependent SE measurements the real part $<\varepsilon_1>$ of the pseudodielectric function is determined at 3.5 eV (see Fig. 1a). The energy of 3.5 eV is selected because it is close to the optical absorption edge of $K_{0.85}Na_{0.15}NbO_3$ which makes the dielectric constant sensitive to any structural change. The clearly visible kink indicates a structural modification in the film, while the substrate shows constant values in the whole temperature range. The pronounced discontinuity at 428 K can be attributed to the phase transition in the $K_{0.85}Na_{0.15}NbO_3$ film from the monoclinic M_c-phase, characterized by periodic arrangement of stripe domains, to the orthorhombic c-phase with irregularly arranged ferroelectric domains (corresponding unit cells and domain structures are shown as insets in Figs. 1a). The refractive index *n* and the extinction coefficient *k* for the monoclinic and orthorhombic phases are now evaluated at temperatures below (RT) and above (523 K) the phase transition, respectively, by B-spline fitting of the ellipsometric angles Ψ and Δ as a function of energy (see Fig. 1b). While in the energy range up to ~3.5 eV the extinction coefficient *k* is close to zero indicating a transparent region, the refractive index *n* slightly increases from 2.2 to about 2.5 for both phases.

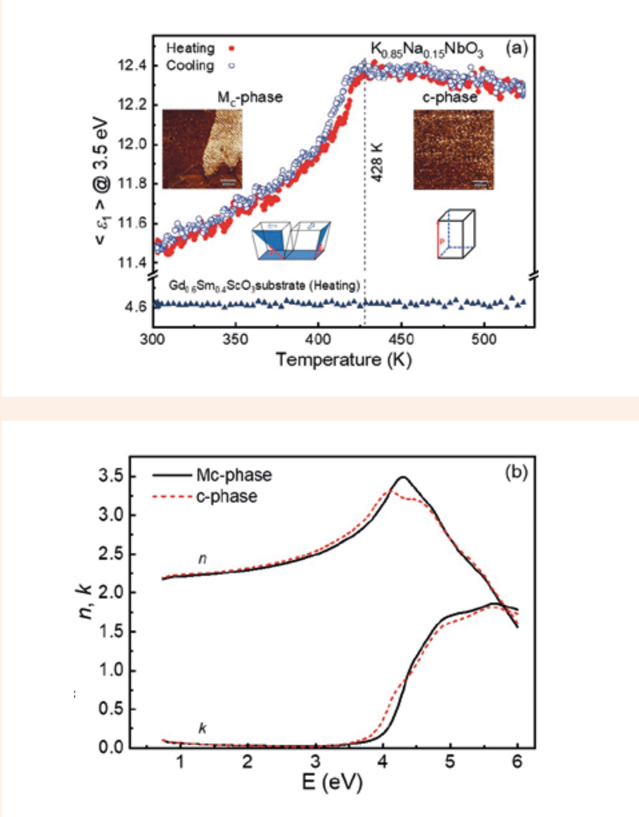

Fig. 1 (a) Temperature dependent spectra of the real part of the pseudodielectric function $<\varepsilon_1>$ of the $K_{0.85}Na_{0.15}NbO_3$ film and the $Gd_{0.6}Sm_{0.4}ScO_3$ substrate. Inset, lateral piezoresponse force micrographs (amplitude images) and the orientation of the polarization vector direction within the unit cell of the M_c- and c-phase.
(b) Refractive index *n* and extinction coefficient *k* as a function of photon energy in the M_c-phase (black line) and c-phase (red, dotted line) for the epitaxial $K_{0.85}Na_{0.15}NbO_3$ film.

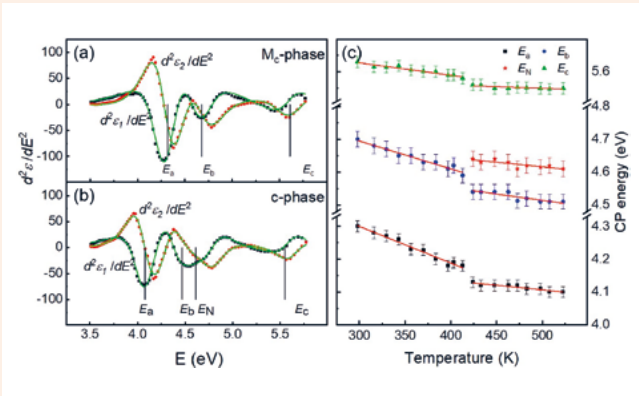

Fig. 2 Second derivatives of ε_1 and ε_2 in the M_c-phase (a) and c-phase (b). Temperature dependence of the threshold energies E_a, E_b, E_N and E_c of the $K_{0.85}Na_{0.15}NbO_3$ film (c).

A strong increase in k displays the onset of absorption at higher energies, which also results in an increase of *n* until a maximum is obtained at ~4.5 eV. Fig. 1(b) also indicates that in the transparent region (< 3.5 eV) *n* and *k* are quite similar for the monoclinic and the orthorhombic symmetry, but strong differences exist in the absorption range (> 3.5 eV).

The optical band gaps are deduced from Tauc plots, where the low energy part of the measured absorption coefficients is fitted with a power function resulting in indirect band gaps of (3.75 ± 0.02) eV and (3.60 ± 0.02) eV at room temperature (M_c-phase) and 523 K (c-phase), respectively. This obvious redshift of the absorption edge is due to temperature-dependent dilatation of the lattice, polarization effects and electron-lattice interaction [3]. A further significant difference between the M_c- and c-phase is evident in the refractive index and extinction coefficients of the absorption range, where several local maximam and minima can be observed (see Fig. 1b). These local extrema are typically referred as critical points and are related to electronic interband transitions. By using a standard critical point analysis of the 2nd derivatives $d^2\varepsilon/dE^2$ of the dielectric function we could identify three interband transitions for the M_c-phase (see Fig. 2a). The corresponding energy positions are indicated by the black lines and labeled as E_a, E_b, and E_c in the order of increasing photon energy. However, for the c-phase significant energy shifts for E_a, E_b, and E_c and an additional critical point denoted as E_N are observed (Fig. 2b). This is more obvious in Fig. 2(c), where the temperature dependency of the interband transition energies are shown. For all critical points, with increasing temperature a systematic redshift can be observed caused by temperature-dependent electron-phonon interactions, while the occurrence of discontinuities at the phase transition temperature are attributed to shifts of the Nb atom in the NbO_6 octahedron during phase transition. This affects the orbital hybidization and leads to appearance of an extra electronic transition.

Our results indicate that optical properties and electronic transitions are very sensitive to structural variations at the phase transition of ferroelectric perovskite oxide materials.

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Gallium oxide substrate *Photo: Volkmar Otto*

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Step-flow is all you need: Mitigating the morphological instability

This report is based on the following publications [1] and [2]

Our modern society relies on a multitude of electrical and electronic systems. The majority require the conversion of one form of electricity into another in order to make the energy usable. According to a report (Bericht 2021 AG Energiebilanzen e.V.), 65% of the energy generated in 2021 was lost mainly through power conversion, flare, and line losses. Efficient power electronics are therefore essential and a decisive factor in the energy transition. The new semiconductor material, beta-gallium oxide (Ga_2O_3) has the potential to reduce these conversion losses, cut costs, and thus make a significant contribution to climate protection. Ga_2O_3 is particularly promising for high-voltage applications, typically up to the 10 kV level or above.

These applications require high-quality β-Ga_2O_3 epiwafers (wafer + epitaxial layer as the electrical active part of a device), preferably grown by metal-organic vapor phase epitaxy (MOVPE) as an industrial compatible method, with precise control over the thickness and doping concentration, ideally in a vertical device structure. Maintaining morphological stability (step-flow growth) is crucial for minimizing structural defects in the epilayer across a wide range of thicknesses and doping concentrations. A step-flow instability manifests mainly in two phenomena: i) step meandering and ii) step pinning. This article investigates both phenomena and provides a solution to maintain the step-flow morphology during growth, thereby realizing high-quality layers with respect to both structural and electrical properties.

i) Step-meandering [1]

Homoepitaxially grown Ga_2O_3 layer with several µm layer thickness are used as the drift layer in vertical devices. To avoid the formation of twin lamellae, which harm the electrical properties, a periodic step-and-terrace morphology (step-flow growth) is essential. However, the presence of a potential wall at the step edges on the vicinal growth surface, the Ehrlich-Schwoebel Barrier (ESB), disrupts step uniformity by restricting the free exchange of surface Ga adatoms between terraces, leading to step instabilities.

Under high O_2/Ga ratio growth conditions the ESB induced surface kinetic instabilities for the gallium adatoms. This leads to a morphological evolution transition in growth mode from step-flow growth via step meandering (Figure 1a) to rough step-bunching as the thickness increases (>350 nm under the reported conditions). This morphological transition is irreversible and significantly degrades the electrical properties of the grown film. Transmission electron microscopy images further confirm variations in step heights and provide direct evidence of these instabilities.

To increase the step stability, an adjustment of the O_2/Ga ratio is necessary. Our assumption is that an increase in the Ga flux (while keeping O_2 constant) results in the formation of a Ga-adlayer on the growth surface, which enhances surface diffusion, mitigates step perturbations, and stabilizes the step-flow growth. By optimizing the O_2/Ga ratio accordingly, µm-level thick (100) β-Ga_2O_3 films with stable step-flow morphology (Figure 1b) and high carrier mobility were successfully achieved.

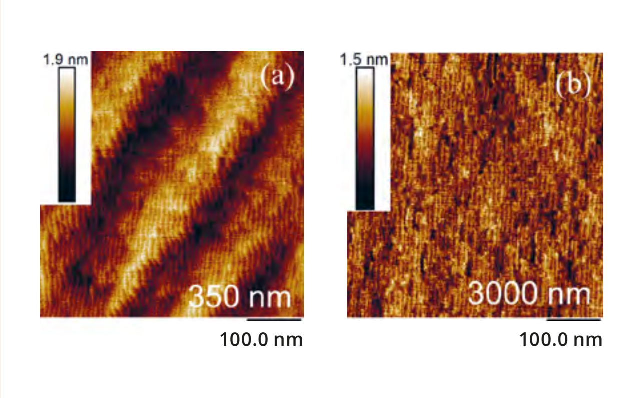

Fig. 1 AFM image of a homoepitaxially grown (100) β-Ga_2O_3 film, showing (a) step-meandering under high O_2/Ga ratio growth conditions at a 350 nm thickness and (b) stable step-flow under low O_2/Ga ratio growth conditions up to 3000 nm thickness. (Reprinted from Ref. [1])

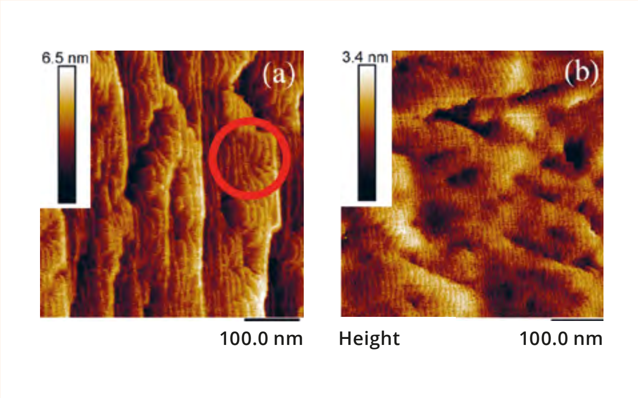

Fig. 2 AFM images of homoepitaxially grown (100) β-Ga_2O_3 film, showing (a) step-pinning-induced curved step-bunching under a high O_2/Ga ratio growth condition and (b) recovered step-flow under a low O_2/Ga ratio growth condition both at a doping concentration of 10^{18} cm^{-3}. (Reprinted from Ref. [2])

ii) Step-pinning [2]

Si is widely utilized as an effective n-type dopant in β-Ga_2O_3 epitaxial films. However, at high doping concentrations (>10^{18} cm^{-3}), Si can significantly affect growth dynamics by altering local gallium (Ga) supersaturation, particularly under conditions of low Ga supersaturation (high O_2/Ga ratio). Since Si atoms act as adsorption sites, Si affects the growth dynamics, reducing the availability of Ga adatoms and subsequently decreasing the step velocity by pinning the step. This disruption in step-flow growth results in irregular step formation, particularly the development of curved steps, as highlighted in the red circle in Figure 2a. It also leads to growth stalling and, ultimately, step bunching – aligning with predictions from the Cabrera–Vermilyea model, which describes impurity-induced step-pinning effects. Uncontrolled step bunching can introduce structural defects and degrade the electrical properties of β-Ga_2O_3 films, underscoring the need for precise control of doping levels and growth conditions.

Since the MOVPE process under the used conditions is a mass-transport-limited process, a proven strategy to mitigate step pinning and restore step velocity is to significantly enhance Ga supersaturation. This can be achieved by increasing the Ga precursor flux to decrease the O_2/Ga ratio near to the Ga-rich boundary (similar to the case of step-meandering). This results in a stable step-flow morphology (Figure 2b) and high-quality epitaxial layers at a wide range of doping concentration from 10^{16} cm^{-3} to 10^{19} cm^{-3}.

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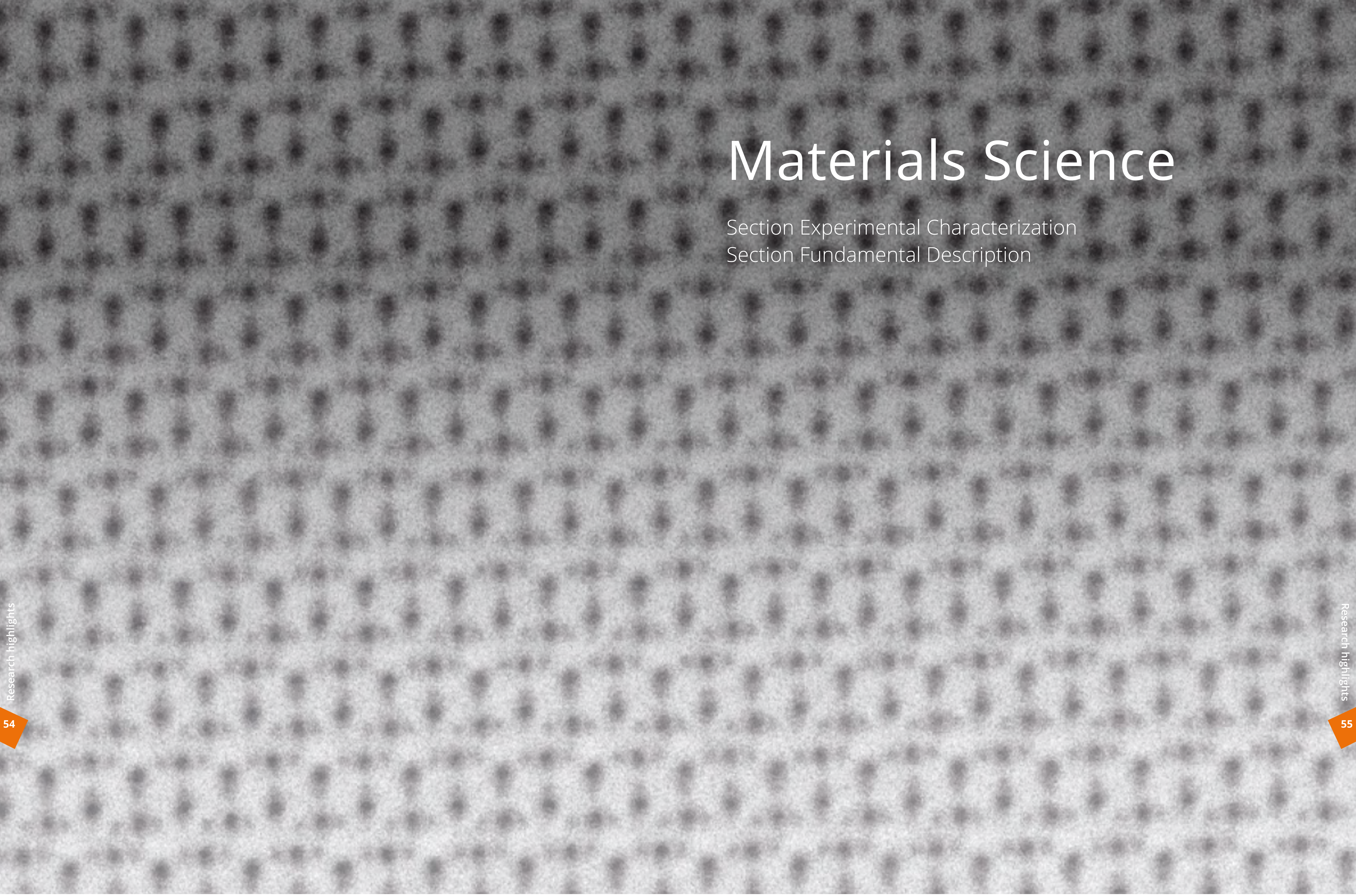
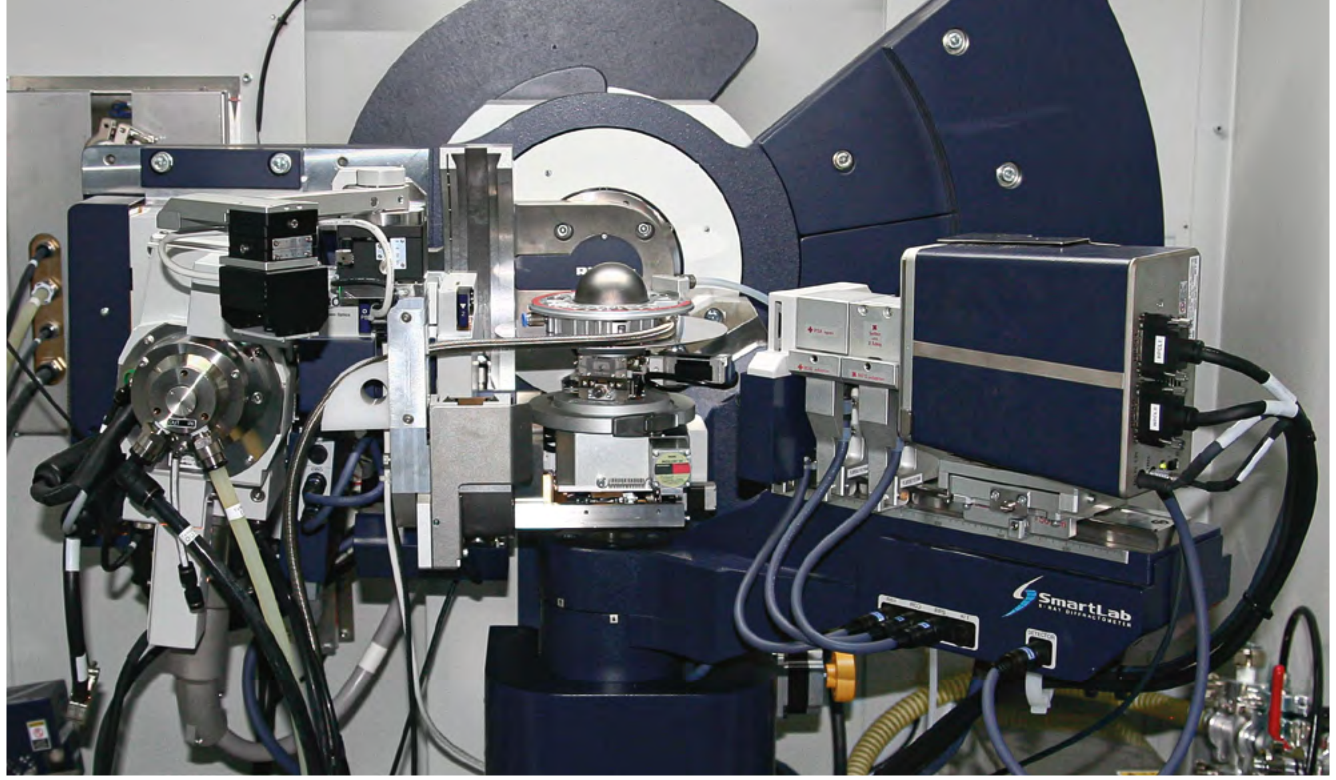


Materials Science

Section Experimental Characterization
Section Fundamental Description

IKZ Annual Report 2024



SmartLab X-ray diffractometer *Photo: IKZ*

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Periodic lateral superlattice in bonded $SrTiO_3/SrTiO_3$ twisted perovskites verified by X-ray diffraction

The process of stacking free-standing membranes has been demonstrated to facilitate the formation of interfaces that surpass the capabilities of conventional heteroepitaxy. In particular, twisted interfaces provide unique physical properties, not present in the corresponding individual layers. The ideal twist grain boundary is known to yield an in-plane screw-dislocation network under the assumption of sufficiently strong interactions across the interface, for example via covalent or ionic bonding. The distance between the dislocation lines, which is equivalent to the length scale of the Moiré pattern $L_{Moiré}$, is determined by the twist angle φ between the adjacent crystalline surfaces (Fig. 1(a)). The associated strain gradients of the periodic pattern are of particular interest for oxide-based perovskites due to the intricate connection between surface polarization and subtle structural deformations such as oxygen octahedra tilts.

Within DFG-project "nano-twist", the Leibniz-Institut für Kristallzüchtung has developed a transfer bonding process which produces efficient bonding of freestanding $SrTiO_3$ layers to $SrTiO_3$ single-crystal substrates. Our approach involves an epitaxial $SrTiO_3/(Ca,Sr)_3Al_2O_6$ layer system grown on $SrTiO_3$ substrate, which was bonded to a $SrTiO_3$ substrate via an annealing step at high temperature. Thereby the $(Ca,Sr)_3Al_2O_6$ sacrificial layer is water-soluble and was only subsequently dissolved [1]. Film growth and bonding procedures were performed in the sections "Thin Oxide Films" and "Semiconductor Nanostructures".

The twisted $SrTiO_3/SrTiO_3$ interface was investigated by grazing incidence in-plane X-ray diffraction (GIXD) enabling the observation of clear signatures of a highly periodic lateral superlattice consistent with the formation of a screw-dislocation network. The experiment was conducted at the BM25B beamline of the European Synchrotron (ESRF). Further measurements were also undertaken at the PHARAO beamline of BESSY II.

Figs. 2(a) and 2(b) display 2D GIXD diffraction patterns in the vicinity of the 200 and 110 in-plane Bragg reflections, respectively. For both Bragg reflections two strong peaks can be identified which are caused by the film (F) and the substrate (S). Their relative positions prove that film and substrate exhibit identical in-plane lattice parameters and are solely different in the in-plane orientation ('twist') which in the present case is φ = 0.80°.

In addition to the two main peaks, weak but sharp satellite reflections are identified, which form a two-dimensional square lattice aligned along the Q_{100} and Q_{010} in-plane directions. Both the orientation and the period (ΔQ) of the square lattices are identical for both Bragg reflections, i.e., independent of the Q-vector. Therefore, a periodic structure with a well-defined in-plane supercell with dimension $L = 2\pi/\Delta Q = 27$ nm must have formed at the interface between substrate and layer. Furthermore, the square satellite pattern is symmetrical to the substrate (S) and film (F) reflections. This proves that the superstructure is commensurate with the film and substrate atomic lattices. The prerequisite for the formation of such a superlattice is the presence of chemical bonds at the interface, which necessitates structural relaxation by the formation of screw-dislocations.

Due to the macroscopically homogenous film and substrate, we expect equidistant screw-dislocations – as schematically depicted in Fig. 1(b) – and thus the generation of a periodic network at the interface with a period of $L_{Moiré} = (a/2) / \sin(\varphi/2)$. Using a lattice parameter of a = 3.905 Å and a twist angle of φ = 0.80° we obtain L = 28 nm in excellent agreement with the value derived from the GIXD satellite pattern.

The distortion field of the buried dislocation network is not solely located at the film-substrate interface. Rather, it gradually decays perpendicular to the film/substrate interface. In order to obtain a detailed view of this complex strain scenario, the Extended Finite Element Method (XFEM) has been utilized to calculate the full 3D strain tensor ε_{ij}. In the simulation, we assume an ideal twist boundary with a periodic network of pure screw-dislocations. These are buried 10 nm below the surface of the sample with in-plane Burgers vectors and corresponding dislocation lines along [100] and [010]. Therefore, the only strain components to be expected are shear strains. All normal components (ε_{11}, ε_{22} and, ε_{33}) are essentially zero throughout. In Fig.3, the in-plane shear component ε_{12} is displayed. This component is strongest directly at the interface and effectively penetrates into the underlying substrate and twisted film.

The observed rotational Moiré pattern is exclusively originated from an in-plane twist between the film and substrate, which exhibit identical in-plane lattice parameters. No significant out-of-plane tilt angle of the bonded thin film with respect to the substrate was observed. Consequently, it is expected that the dislocations at the interface will be of a pure screw type with in-plane Burgers vector.

The present work represents a collaboration between the sections "Thin Oxide Films", "Semiconductor Nanostructures" and "Experimental Characterization" as well as the Paul-Drude-Institute Berlin. Our results demonstrate a robust route for the fabrication of twisted perovskites and their development into a functional material platform with targeted strain gradients on the nanoscale.

We thank ESRF (experiment HC-5796) and DFG for funding "nano-twist" (MA 9075/1-1, SCHW 1500/9-1).

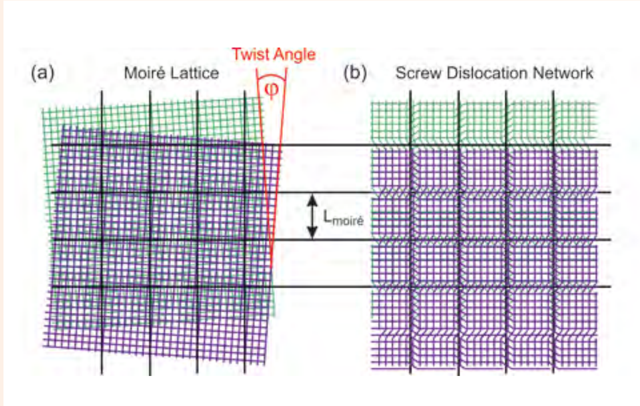

Fig. 1 (a) Formation of a periodic Moiré pattern by the overlay of two twisted square lattices with identical lattice parameters. (b) Schematic of a periodic screw dislocation network at the interface showing a square supercell with dimension of $L_{Moiré}$ (adapted from [1].)

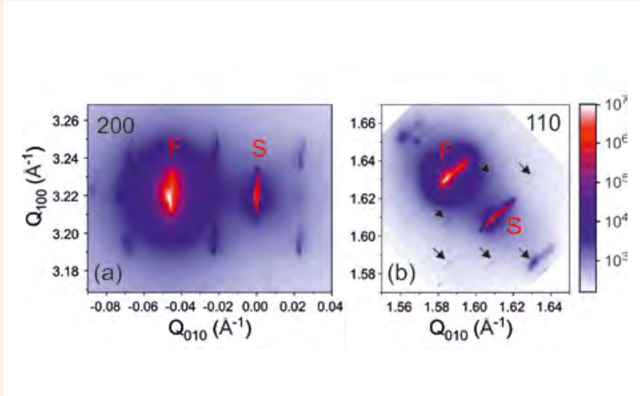

Fig. 2 Grazing incidence in-plane X-ray diffraction (GIXD) patterns in the vicinity of the (a) 200 and (b) 110 $SrTiO_3$ in-plane Bragg reflections. The substrate and film peaks are marked as 'S' and 'F', respectively (adapted from [1]).

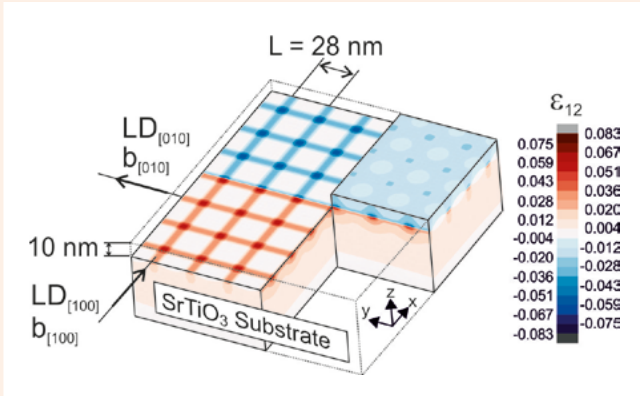

Fig. 3 Simulation of the in-plane strain component ε_{12} derived from the Extended Finite Element Method for a 10 nm $SrTiO_3$ twisted thin film on $SrTiO_3$ substrate (φ = 0.80°). We assume an orthogonal periodic array of pure screw-dislocations buried 10 nm below the sample surface and aligned along the <100> line directions (LD). The left-hand side of the figure depicts the areas situated directly below and above the interface, while the right-hand side illustrates the situation at the surface. Vertical planes situated at the dislocation core (y-z-plane) and between two adjacent dislocation lines (x-z-plane) provide a detailed insight into the vertical decay of ε_{12} (adapted from [1].)

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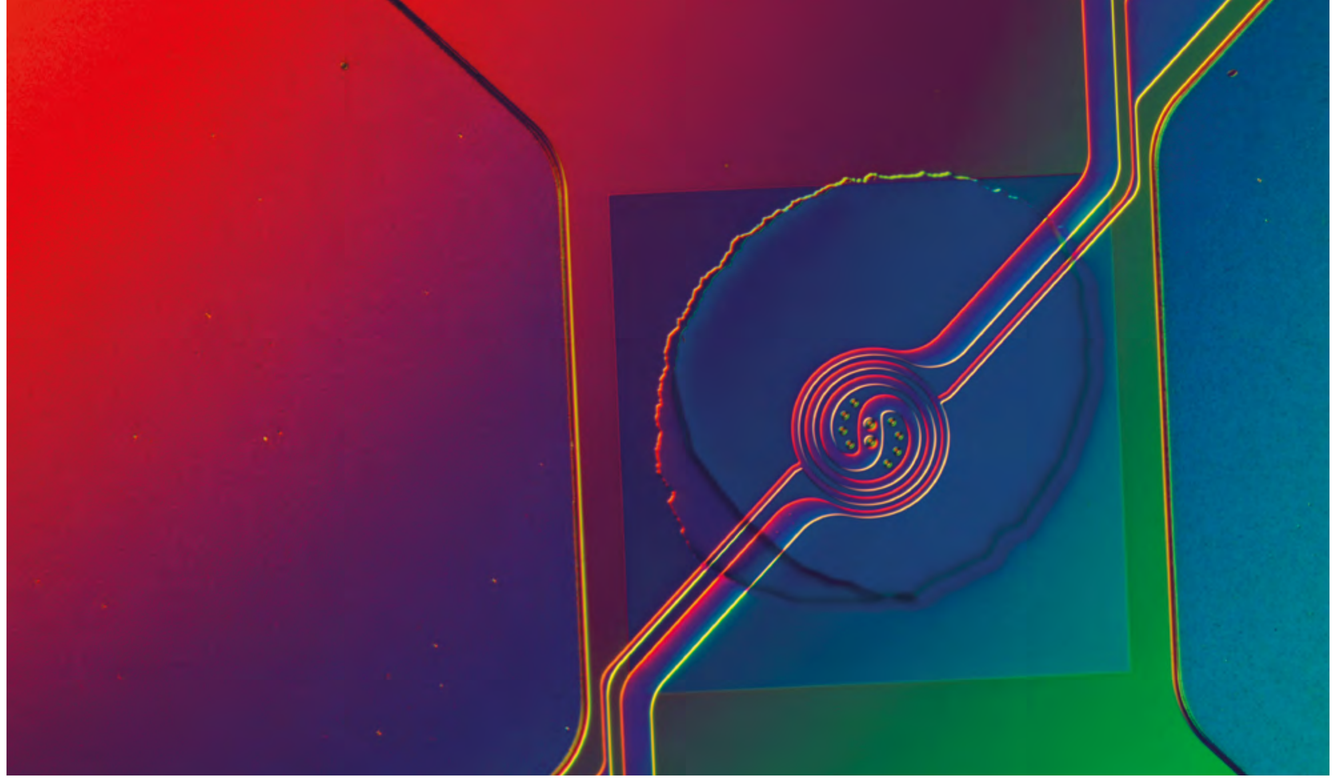

Amorphous Ga_2O_3 on a MEMS chip (TEM image) *TEM image: IKZ*

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Unraveling the atomic mechanism of the disorder–order phase transition from γ-Ga_2O_3 to β-Ga_2O_3

Gallium oxide (Ga_2O_3) has emerged as a novel semiconductor material, offering exceptional properties such as an ultra-wide bandgap (4.7 eV) and a high breakdown electric field (8 MV/cm). The possibility to grow it from the melt holds the promise for cheap, large diameter substrates. These characteristics make it a prime candidate for next-generation high-power electronics, solar-blind UV photodetectors, and radiation-resistant devices. However, the material's polymorphic complexity – existing in multiple metastable phases (α, β, γ, κ, δ) alongside its stable monoclinic β-phase, while offering interesting heterostructures for device applications – has posed significant challenges for researchers.

A joint study by the Leibniz-Institut für Kristallzüchtung and the Paul-Drude-Institut in the framework of the Leibniz Science Campus GraFOx has provided an atomic-level description of the most technologically relevant transformation, namely the conversion of the cubic spinel-type γ-phase into the ordered monoclinic β-phase that takes place after doping implantation and recovery after annealing. We followed crystallization of amorphous Ga_2O_3 films, deposited by molecular beam epitaxy on a MEMS heater chip, inside a transmission electron microscope while ramping the temperature from room temperature to 1000 °C (Fig. 1). At 470 °C the diffuse diffraction halos of the amorphous phase sharpened into Debye Scherrer rings characteristic of γ-Ga_2O_3; continued heating brought a progressive change in diffraction intensities indicating the presence of γ-Ga_2O_3 β-type pattern. At 950 °C, an entirely β-type pattern was observed. The continuous nature of the intensity evolution over a wide temperature range identifies the transformation as a second-order, disorder-to-order process rather than an abrupt martensitic change.

The key to this behavior is a shared structural scaffold (Fig. 2). Both polymorphs possess an almost identical face-centered-cubic oxygen sublattice. In γ-Ga_2O_3 (Fig. 2b) roughly twenty percent of the gallium atoms occupy interstitial positions within four symmetry-related tunnels of β-Ga_2O_3, leaving an equal number of vacancies on the regular sublattice; β-Ga_2O_3, by contrast, is fully ordered (Fig. 1a). By superimposing the two lattices we constructed a coincidence-site model that reveals how the γ structure can be regarded as a defective variant of the β phase. During annealing, misplaced

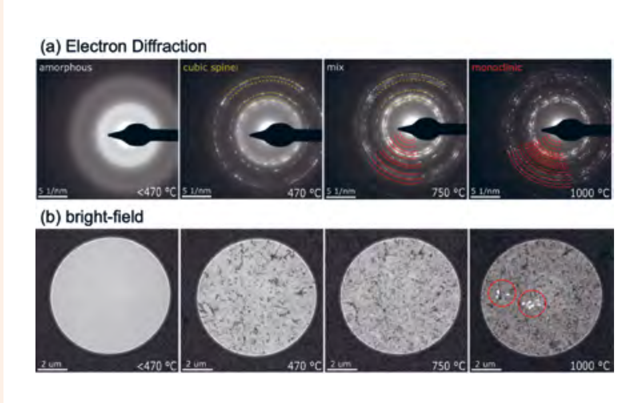

Fig. 1 (a) Electron diffraction pattern visualizing the crystallization process of Ga_2O_3 upon annealing to higher temperatures. Gold and red arcs represent the Debye–Scherrer rings referred to the hkl reflections of the cubic spinel and monoclinic phases, respectively. The black feature in the center is the beam stop to prevent damage of the scintillator of the camera. (b) Bright-field images of the crystallized films upon annealing. Dark areas represent crystallites that fulfill Bragg conditions. The areas highlighted by the dashed circles at 1000 °C indicate the effect of the beam on the samples.

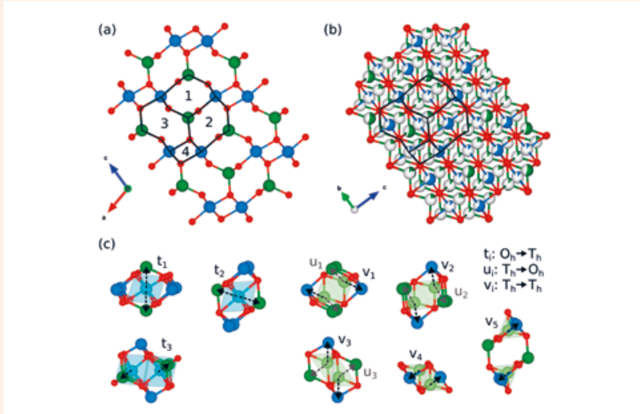

Fig. 2 Equivalent projected volumes of (a) the β-Ga_2O_3 crystal structure in [010] projection and (201) out-of-plane orientation with four inequivalent empty tunnels indicated and (b) the γ-Ga_2O_3 crystal structure in [110] projection and (111) out-of-plane orientation with the partial occupation of lattice sites indicated by partly colored balls. (c), the interstitials defined in the different tunnels in panel are identified as octahedral (blue) and tetrahedral (green) interstitial sites in the β lattice. The different atomic jumps needed to transition from the γ phase to the β phase are indicated by arrows and labeled as t_i, u_i, and v_i.

gallium cations hop from octahedral or tetrahedral interstitials into the adjacent vacancies, step by step reducing the configurational entropy while preserving the oxygen framework (Fig. 2c). Because each hop must surmount a local energy barrier that depends on the surrounding defect configuration, the collective rearrangement extends over a broad temperature window – a behavior perfectly reproduced by the in-situ data.

Experiments on Ga_2O_3 layers grown epitaxially on sapphire corroborated the microscopic picture. On a crystalline template the nascent γ grains adopt a fixed orientation relationship with the substrate; as the disorder subsides the grains convert coherently into equally well-oriented β domains.

These insights have immediate technological consequences. During ion implantation – an essential step for introducing donor or acceptor species – the β lattice often collapses locally into γ-like fragments. The present study shows that a moderate post-implant anneal suffices to drive the reverse migration of gallium and to restore the β order, thereby providing a clear protocol for damage recovery and dopant activation. The same γ↔β pathway also accounts for the remarkable radiation tolerance reported for Ga_2O_3: the crystal can absorb high defect loads in the γ configuration and subsequently heal itself without amorphizing.

Important challenges remain. Traditional density-functional calculations struggle with the statistical site occupancy that defines γ-Ga_2O_3; advanced cluster-expansion and machine-learning approaches will be required to predict defect energetics, diffusion barriers and dopant interactions with comparable precision. A deeper understanding of how intentional impurities influence phase stability could unlock phase-engineered heterostructures and novel switching concepts based on controlled polymorphic transformations.

Nevertheless, the present work provides a rigorous experimental benchmark and a coherent mechanistic framework that turn gallium-oxide polymorphism from a liability into a design parameter. By bridging atomic-scale processes and macroscopic behavior, it lays the foundation for reliable Ga_2O_3 electronics capable of operating under the extreme voltages, temperatures and radiation levels demanded by tomorrow's power converters, ultraviolet detectors and space-borne sensors.

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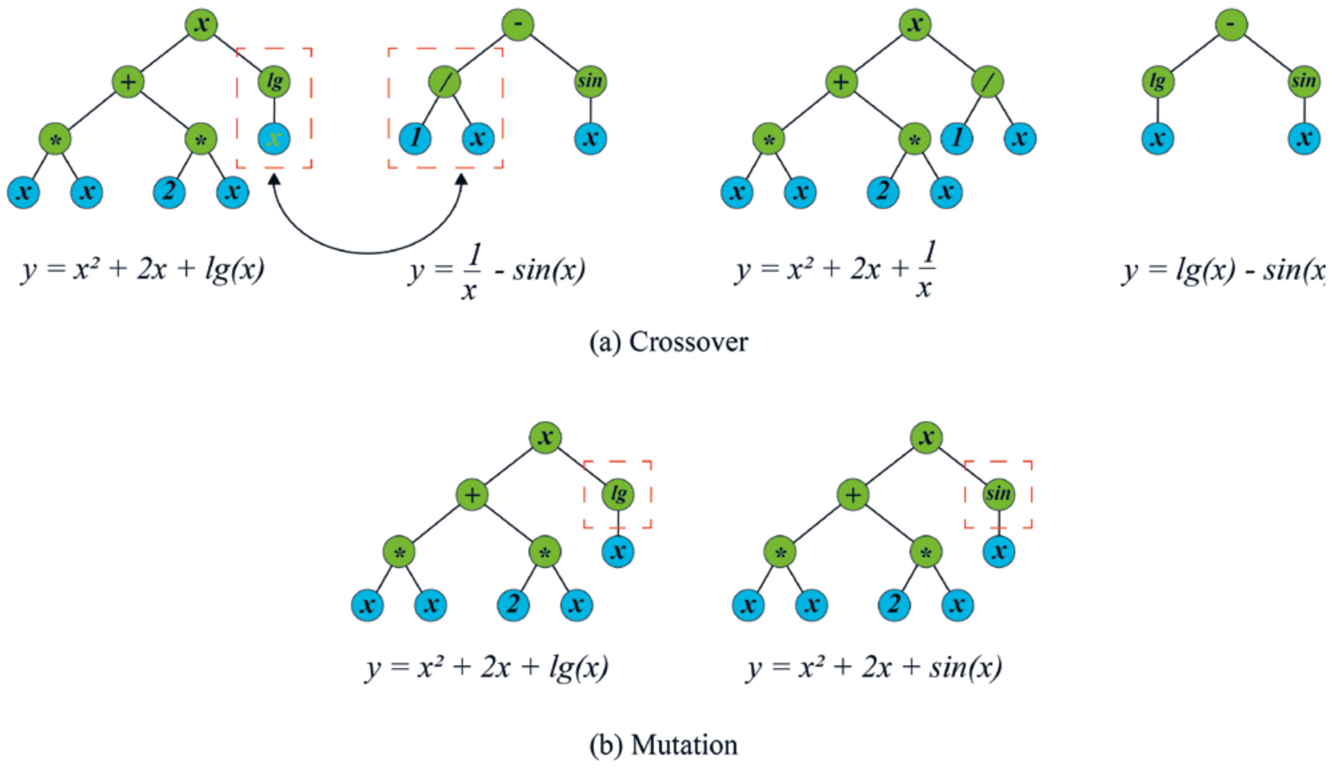

Illustration of symbolic regression using genetic programming: ex-pressions are represented as trees and evolved through crossover and mutation to discover interpretable mathematical models *Image: IKZ*

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SyMO: a hybrid framework for multi-objective optimization of Cz-Si

The Czochralski (Cz) method remains a cornerstone in the production of high-purity, monocrystalline silicon, crucial for semiconductor and photovoltaic applications. Optimizing this complex process is essential to improve crystal quality and manufacturing efficiency. Challenges in the Cz method include managing temperature gradients, interface morphology, and defect concentrations, all of which are sensitive to a wide range of interrelated process parameters and furnace configurations. Traditional optimization approaches, based on either experimental trial and error method or computational fluid dynamics (CFD), are limited by high cost and poor generalizability.

To address these limitations, we developed SyMO – a Symbolic regression-based Multi-Objective optimization framework (Figure 1). This hybrid methodology combines CFD simulations, machine learning (symbolic regression), and mathematical optimization to explore and optimize the silicon crystal growth process in a rigorous and interpretable manner.

Symbolic regression (SR) in the SyMO framework leverages evolutionary computation techniques to discover analytical expressions that model complex relationships between process parameters and crystal quality metrics. Unlike conventional machine learning models, which are often considered "black box," SR generates interpretable mathematical expressions. These expressions are composed from a predefined set of functions and operators – such as logarithms, exponentials, powers, ReLU (Rectified Linear Unit), and sigmoids – chosen based on domain knowledge to reflect realistic physical behaviors.

In our study, the SR algorithm is implemented using PySR, an open-source library designed for symbolic regression in scientific applications. PySR employs a multi-population evolutionary search strategy with configurable complexity constraints to balance model expressiveness and interpretability. Operators are assigned individual complexity scores, and nesting is restricted to avoid overly convoluted expressions that lack physical meaning.

The SR models evolve over multiple generations, where each generation involves a process of selection, crossover, and mutation - analogous to biological evolution. Candidate models with lower prediction error (typically measured by Root Mean Squared Error or RMSE) are selected to form the basis for the next generation. Crossover operations combine segments of two parent models to produce new variants, while mutations introduce random changes to encourage diversity in the search space. The fittest models are preserved or refined in subsequent iterations, gradually converging toward optimal expressions.

The SyMO workflow begins with the generation of a comprehensive dataset using quasi-steady-state, axisymmetric CFD simulations. These simulations capture the heat and momentum transport phenomena during Cz-Si growth in various furnace setups, incorporating different heater placements, radiation shield materials, and process parameters such as pulling rate, crystal and crucible rotation, and power input. The dataset spans 342 unique scenarios, ensuring broad coverage of physically relevant process space.

SR is then used to derive analytical expressions linking fifteen input geometrical and process parameters x1-x15 to two key crystal quality indicators: interface deflection Δz (eq. 1.1-1.3) and the relative Voronkov criterion ΔΓ (eq. 2.1-2.3). Unlike black-box models, SR yields interpretable equations, enabling both accurate prediction and physical insight into the crystal growth process. The derived equations capture non-linear relationships, incorporating exponential, logarithmic, and piecewise behaviors.

The resulting expressions are integrated into a hierarchical multi-objective optimization (MOO) model. The objectives are: minimizing the magnitude of interface deflection, minimizing deviation from the ideal Voronkov ratio, and maximizing the pulling rate. Physical and engineering limits are imposed as constraints. The optimization problem is formulated as a Mixed-Integer Nonlinear Programming (MINLP) task and solved using Gurobi as the backend solver. The SR models demonstrated high predictive accuracy with normalized mean absolute percentage errors (nMAPE) below 10% for both output variables. For interface deflection, the model captured critical threshold behaviors – e.g., the activation of bottom heater power only above a certain threshold-using ReLU functions. For ΔΓ, sigmoid-based terms modeled thermal and rotational interactions effectively.

Optimization results showed significant improvement in process parameters. For one example of fixed geometry shown in Figure 3, optimal solutions achieved nearly a twofold increase in pulling rate (from 0.5 to 0.96 mm/min), while reducing interface deflection from -12.88 mm to -0.25 mm. The ΔΓ values in optimized runs approached the critical value, ensuring defect minimization. Additional CFD simulations validated these predictions, showing more uniform temperature and flow distributions.

The SyMO framework provides a robust, scalable approach to process optimization in crystal growth. Its use of symbolic regression enables transparent decision-making and better alignment with physical principles, which is vital in high-stakes industrial processes. Furthermore, the MOO model supports real-world trade-offs between competing objectives-balancing yield, quality, and operational constraints.

This approach is not only applicable to silicon, but also extendable to other materials such as germanium or compound semiconductors, and could be integrated into digital twin systems for real-time process control. Future work includes expanding the dataset and refining the models with experimental validation and online learning.

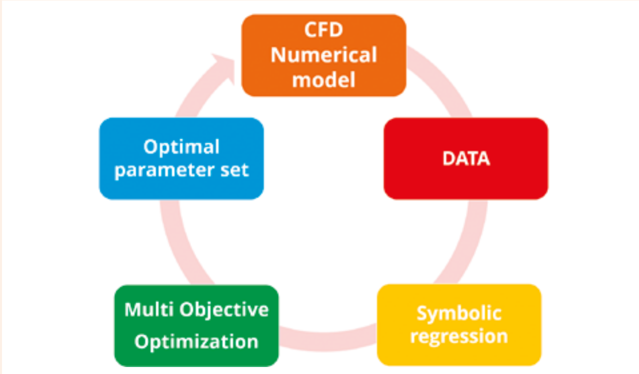

Fig. 1 SyMO framework architecture combining CFD, symbolic regression, and MOO

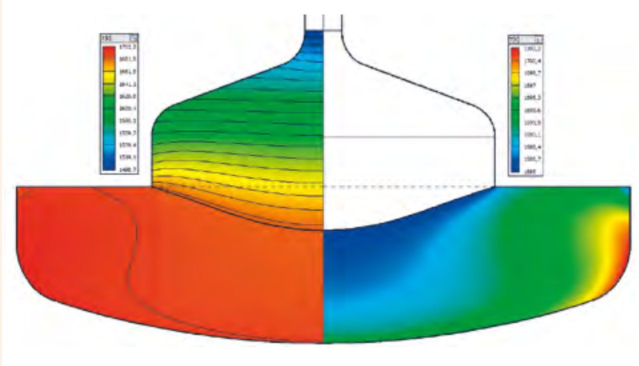

Fig. 2 CFD simulations: temperature and velocity distributions in Si melt and crystal before optimization; more details of this work can be found in [1]

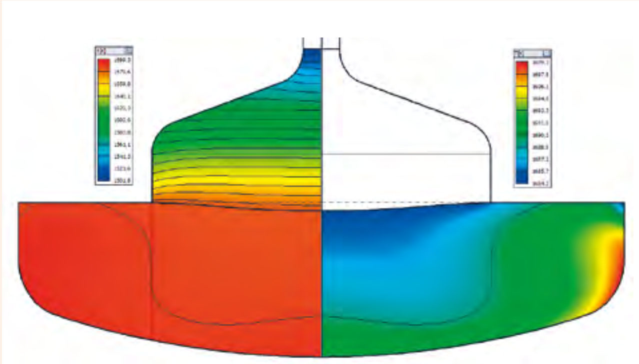

Fig. 3 CFD simulations: temperature and velocity distributions in Si melt and crystal after optimization

$$\Delta z_{\text{term1}} = \sqrt{\text{ReLU}(-25.2277 + x_{15}) \cdot \left| \frac{(x_2 + x_{13})^3 \cdot x_7}{-30.8253 + \frac{x_{14}^6}{(0.8236 \cdot x_1^2 + x_5)^3} + x_{12}} \right|} \cdot e^{x_{13}} \quad (1.1)$$

$$\Delta z_{\text{term2}} = \left(x_{11} + \frac{x_{12}}{\sqrt{\left(\frac{e^{x_{11}/x_9}}{x_1} + x_7 \right)^3}} \right)^2 \quad (1.2)$$

$$\Delta z = (x_{11} + x_4) \cdot \log\left((\Delta z_{\text{term1}} + \Delta z_{\text{term2}})^2 \right) \cdot \sqrt{x_9} \quad (1.3)$$

$$\Delta\Gamma_{\text{term1}} = \left[\text{sigm}\left(0.6114 \cdot |(-2.7649 + x_2) \cdot x_1| \cdot \left(\frac{1}{x_4} \right)^3 \right) \right]^{x_{11}} \quad (2.1)$$

$$\Delta\Gamma_{\text{term2}} = \left(\text{sigm}\left(\frac{x_{14}}{x_6 + \left(\frac{1}{x_{11}^2 \cdot 1.3293} \right) / \left(\left(\frac{x_{13}^2}{x_{12}} + \frac{1}{x_1 - 1.899} \right)^{x_9} \right)^2} \right) \right)^2 \quad (2.2)$$

$$\Delta\Gamma = \left| \frac{\sqrt[3]{x_{11}^2 \cdot \Delta\Gamma_{\text{term1}} \cdot \Delta\Gamma_{\text{term2}}}}{0.2843} \right| \quad (2.3)$$

Fig. 4 Symbolic regression-derived analytical expressions modeling interface deflection and Voronkov critera (v/G), offering interpretable insights for data-driven crystal growth prediction

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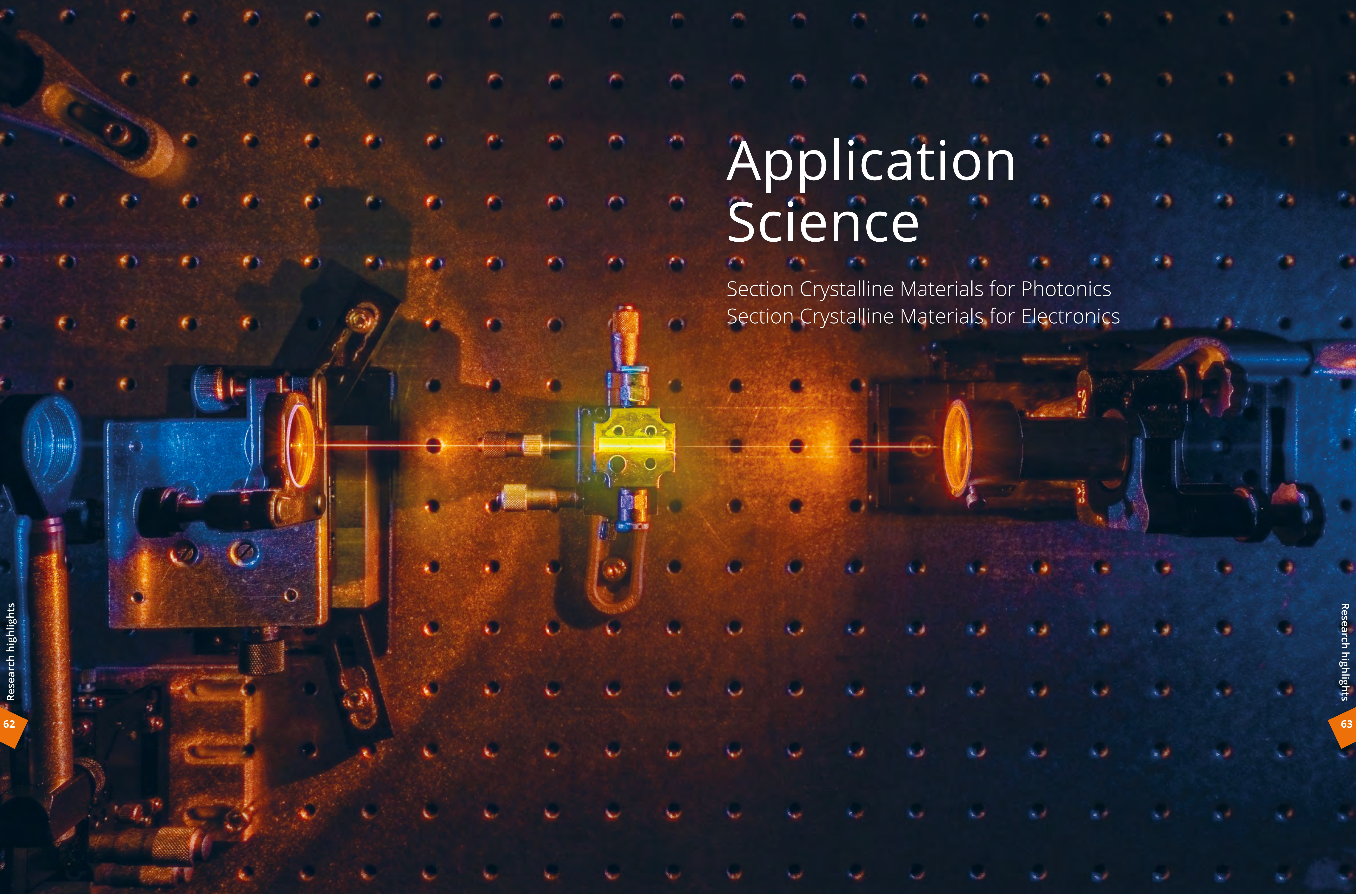
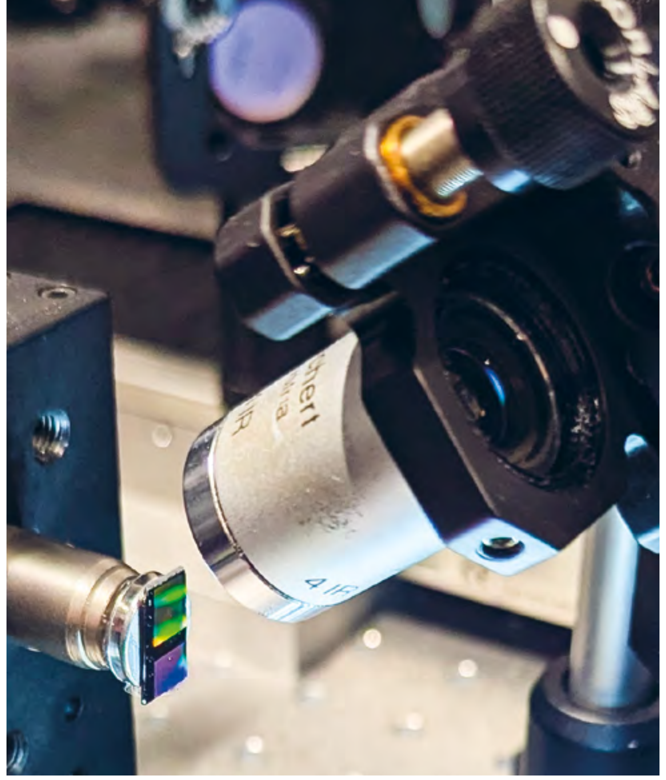
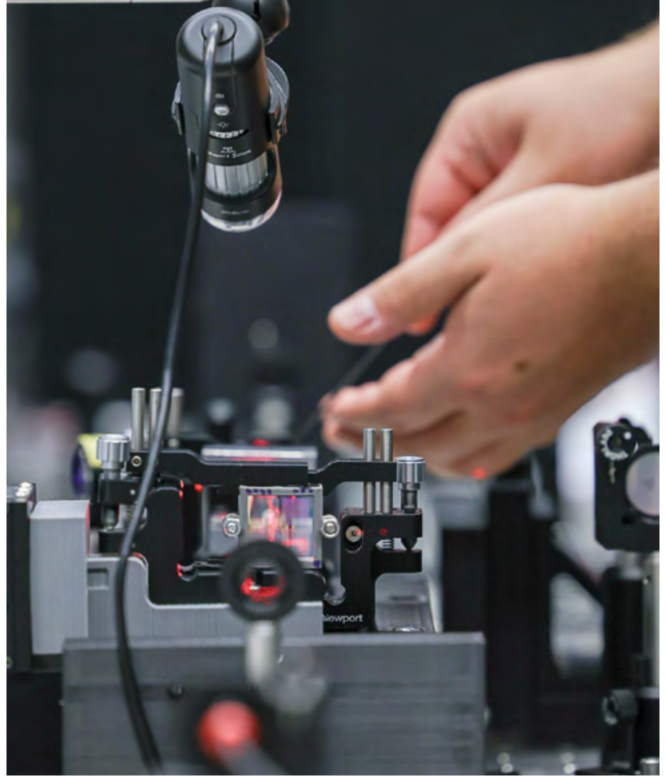


Application Science

Section Crystalline Materials for Photonics
Section Crystalline Materials for Electronics





Left: Nanostructured semiconductor sample mounted in the photoacoustics and time-resolved photoluminescence setup at the IKZ-DESY JointLab.
Rigth: Transient-grating spectroscopy setup for monitoring the propagation of surface acoustic waves in solids *Photo: Peter Gaal, Angela Pfeiffer (DESY)*

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Manipulating the time structure of synchrotron beams

Synchrotron radiation is a type of electromagnetic radiation produced when charged particles, such as electrons, are accelerated to near the speed of light and forced to travel in circular or spiral paths by magnetic fields. It is generated in a special type of particle accelerator, the so-called synchrotron light sources. The synchrotron radiation is highly valuable in scientific research because it is extremely bright and can be finely tuned to different wavelengths, making it ideal for studying materials at the atomic and molecular levels. One of the biggest and most potent synchrotrons in the world is located in Hamburg, Germany. It is called PETRA III and it is operated by DESY, an institute of the Helmholtz Association. IKZ is present on the DESY site with strong research partnership, the IKZ-DESY JointLab.

One of the challenges with synchrotron radiation is its fixed temporal pulse structure. This means that the radiation is emitted in pulses with specific time intervals and durations, which are determined by the operation mode of the synchrotron storage ring. Because synchrotrons host many experiments which are operated in parallel, the operation mode must compromise between the often conflicting needs of different users.

Typically, the emitted pulses have separations ranging from 10 nanoseconds (ns) to 1000 ns and durations of about 100 picoseconds (ps). While this pulse structure is suitable for many experiments, it can limit the flexibility and efficiency of measurements that require different timing configurations (Figure 1).

Active X-Ray Optics: a new tool to modulate the time structure of synchrotron beams

The X-Ray Optics group at IKZ develops different types of active x-ray optics: The WaveGate, which is a fast chopper for selecting individual pulse from the synchrotron pulse train [1]; and the PicoSwitch to shorten the duration of the emitted x-ray pulse [2]. We will focus on the WaveGate in this article.

The WaveGate pulse picker (Figure 2) is a device designed to address this challenge by allowing scientists to tailor the temporal structure of synchrotron radiation to better suit their experimental needs. It works by selectively transmitting or blocking X-ray pulses, effectively reshaping the pulse train emitted by the synchrotron.

The WaveGate consists of two crystals made from a piezoelectric material, which can generate surface acoustic waves (SAWs) when subjected to high-frequency electric fields (Figure 2). These crystals are mounted in a double crystal monochromator (DCM) geometry. The active crystal is equipped with interdigitated transducers (IDTs) that convert the electric fields into SAWs (Figure 3). These waves then modulate the diffraction efficiency of the crystal, allowing it to control the transmission and suppression of X-ray pulses.

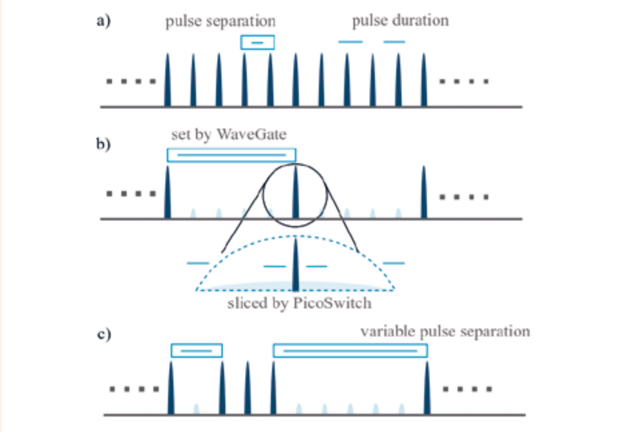

Fig. 1 Typical time structure of synchrotron radiation: a) set by the synchrotron operation mode. b) Modulation with Active X-Ray Optics: the pulse separtion is tailored by the WaveGate and the pulse duration is tailored by the PicoSwitch. c) Example of a modulated pulse spacing for advanced timing measurements.

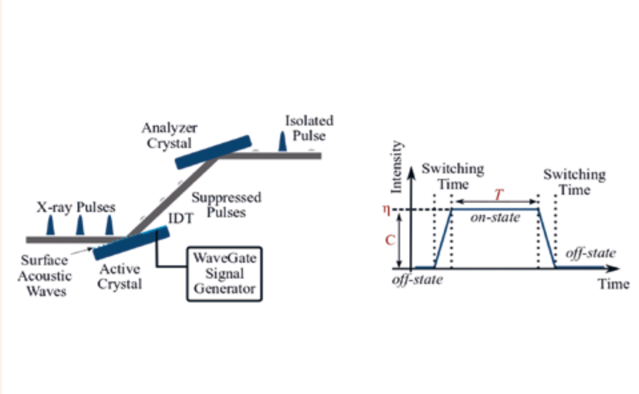

Fig. 2 a) Schematic view of the WaveGate pulse picker. b) WaveGate performance parameters

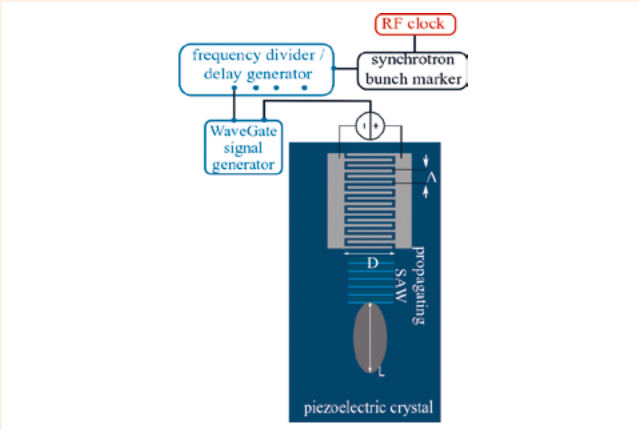

Fig. 3 Layout of the WaveGate active crystal. A high-frequency electronic signal is converted into surface acoustic waves (SAWs) in the piezoelectric substrates. The SAWs propagate towards the impinging x-ray beam (gray area) and generate artificial sidebands to a Bragg reflex.

By adjusting the incidence angle of the X-ray beam and the timing of the SAWs, the WaveGate can diffract the X-ray pulses towards the towards the experiment. By changing the timing of the SAWs, the WaveGate can also suppress the diffraction from the crystals. This process enables precise control over which pulses are transmitted, and which are blocked.

The WaveGate offers several important performance parameters: It achieves a transmission efficiency of over 30% for the incident X-ray beam, meaning a significant portion is successfully transmitted. The device enables switching between transmission and suppression of incoming pulses within 100 nanoseconds to several milliseconds, providing broad temporal control. It features an on-off contrast ratio greater than 10,000, ensuring reliable suppression of unwanted pulses. The WaveGate does not significantly affect the coherence properties of the X-ray beam, which is essential for modern imaging and microscopy applications.

Experiments to characterize the WaveGate's performance were conducted at the KMC3 beamline at BESSY II and the P23 beamline at PETRA III. These experiments involved testing the device with monochromatic X-ray beams at energies of 8 keV and 14.4 keV. Temporal gates with durations ranging from 100 ns to 100 µs were demonstrated, showcasing the flexibility of the WaveGate in adjusting the gate opening time without additional alignment.

The WaveGate was integrated into an optical pump-X-ray probe setup to synchronize optical and X-ray pulses for time-resolved studies. This setup significantly improved the efficiency of measurements by matching the repetition rate of X-ray pulses to that of the optical pump pulses, thus preserving the full dynamic range of the detector.

Additionally, the WaveGate was used to generate complex pulse sequences for advanced timing schemes. These sequences enable the probing of excited systems with predefined pulse patterns, facilitating the retrieval of transient states through linear combinations of measurements.

The WaveGate pulse picker is a versatile tool for temporal shaping of synchrotron beams. It offers high efficiency, flexible timing capabilities, and minimal impact on beam coherence. Its integration into experimental setups enhances the efficiency and flexibility of synchrotron radiation experiments, making it a valuable asset for advanced photonic research. The WaveGate is now commercially available from the IKZ spin-off company TXproducts.

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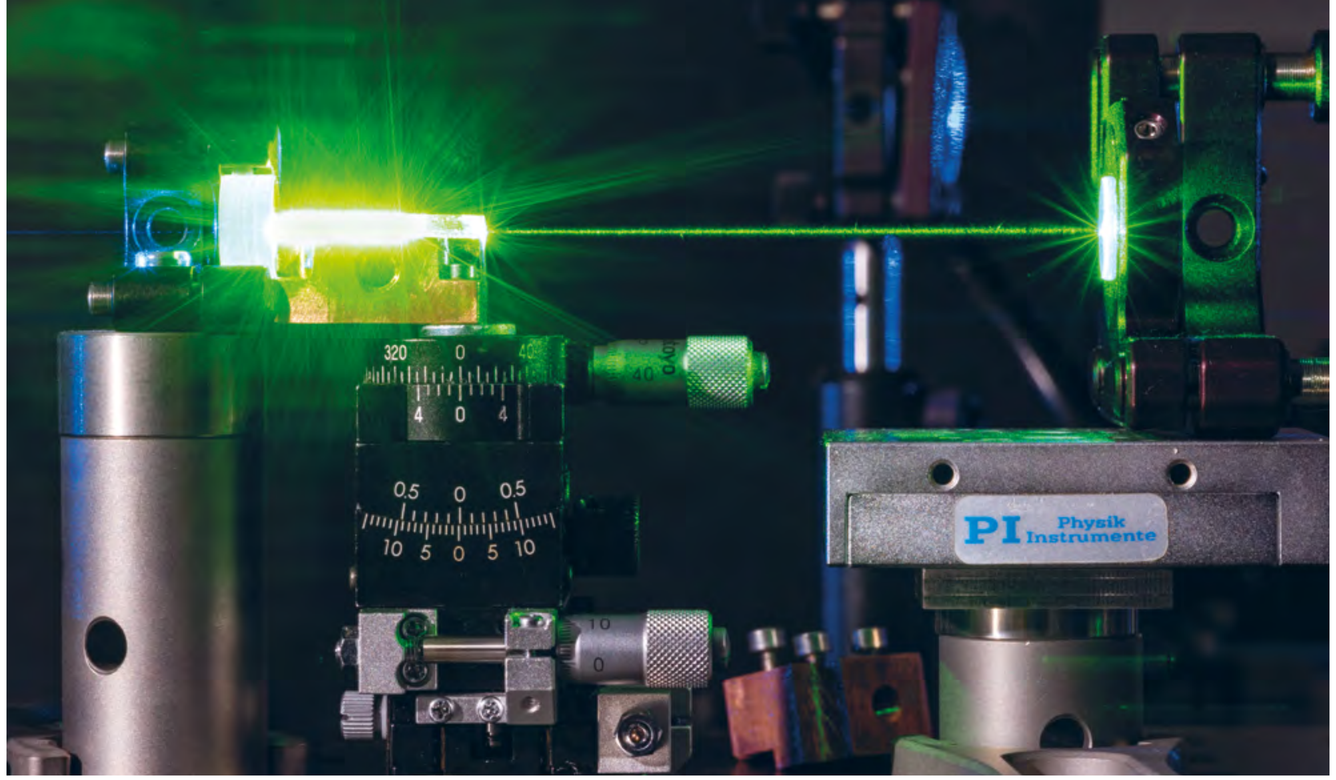

Set-up in the Center for Laser Materials *Photo: IKZ*

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Enhanced laser efficiencies by cryogenic laser operation

Cooling lasers to lower temperatures offers several advantages. One of the most significant benefits is a reduction in the width of the absorption and emission lines, which enhances both absorption and emission efficiency. Narrower transition lines also help to prevent spectral overlap with undesired transitions between energy levels, such as excited state absorption (ESA), cross relaxation (CR), or upconversion (UC), which can cause energy losses and reduce the laser performance.

Moreover, at low temperatures, the thermal conductivity improves and heat dissipates more effectively, and thermal lensing – where thermal expansion and refractive index changes distort the laser beam – can be minimized.

Researchers at the Center for Laser Materials (ZLM) in the Application Science department in cooperation with the mechanical workshop at IKZ thus built an experimental setup capable of operating lasers at temperatures as low as 77 K, the temperature of liquid nitrogen. While using liquid nitrogen for cooling of commercial lasers is rather impractical, thermoelectric Peltier coolers provide a more practical alternative. Even though these do not allow to achieve temperatures as low as those reached with liquid nitrogen, they can cool laser gain materials to temperatures where the efficiency is enhanced while remaining feasible for commercial applications. In fact, many commercial lasers are nowadays enclosed in sealed, dry nitrogen environments to protect against dust and corrosion. Such a dry atmosphere is essential to prevent water condensation during operation at cold temperatures.

ZLM's research takes a modern approach by placing the entire laser resonator inside a vacuum chamber equipped with a liquid nitrogen cryostat to cool the laser sample as shown in Fig. 1. This eliminates losses at chamber windows, which can be an issue in other cryogenic laser setups. To ensure precise alignment at all times, all relevant resonator components are mounted on remote-controlled stages. This setup enables systematic studies of how different laser materials perform at various temperatures.

As a proof of concept, ZLM researchers investigated the performance of a praseodymium-doped yttrium lithium fluoride (Pr^{3+}:$LiYF_4$ or Pr:YLF) laser crystal emitting orange laser radiation at wavelengths of 604 nm or 607 nm. As shown in Fig. 2, the trivalent rare-earth ion praseodymium (Pr^{3+}) has an energy level structure well-suited for visible lasers. When pumped with blue (444 nm) or cyan-blue (479 nm) light, the upper laser level $^3P_0$ is populated, allowing for laser emission at multiple visible wavelengths – ranging from cyan-blue to deep red – depending on the reflectivity of the cavity mirrors. A major challenge for the orange laser transition is orange ground state absorption (GSA), where laser photons are reabsorbed in the gain medium, reducing the laser efficiency. As seen in Fig. 2, the laser wavelength overlaps with an GSA transition in the orange, causing losses for

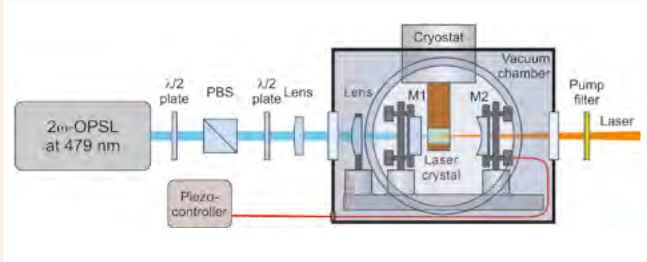

Fig. 1 Setup of the liquid-nitrogen cooled laser (PBS: Polarizing beam splitter, M1: Pump mirror, M2: Output coupling mirror).

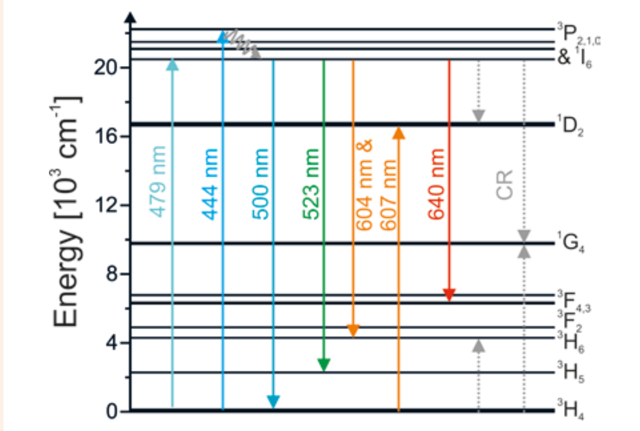

Fig. 2 Energy level scheme of Pr:YLF. Up- and downward arrows indicate absorption and emission, respectively. The wavy grey arrow indicates phonon relaxation, and dashed arrows possible cross-relaxation (CR).

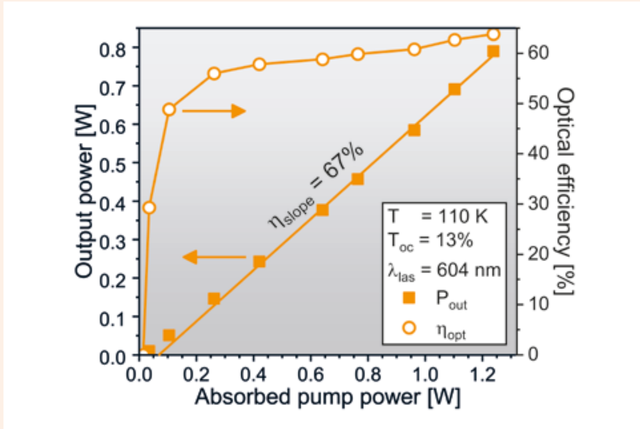

Fig. 3 Orange laser characteristics of a cryogenically cooled 4.7 mm long Pr(0.5%):YLF crystal.

the laser. Cooling the gain medium is suggested to mitigate this issue by narrowing the spectral lines and thus reducing the overlap of laser line and GSA, which should improve the laser efficiency.

In temperature-dependent laser experiments ZLM researchers showed, that the efficiency of orange-emitting Pr:YLF lasers at room temperature is in fact limited by energy losses due to orange GSA [1]. This reabsorption originates from higher-energy Stark levels of the $^3H_4$ ground state, whose population decreases with temperature. At sufficiently low temperatures, the GSA reabsorption vanishes, allowing for record-breaking performance of orange Pr^{3+}-lasers.

Under pumping with a frequency-doubled optically pumped semiconductor laser (2ω-OPSL) at a crystal temperature of 110 K, an impressive slope efficiency of 67% was recorded (see Fig. 3). The laser threshold was reduced by more than an order of magnitude, enabling a record-high optical-to-optical efficiency of up to 64%. At temperatures around 250 K achievable with Peltier cooling, similar slope efficiencies of up to 66% were reached, but due to higher laser thresholds, the optical-to-optical efficiency did not exceed 45% at the available pump power. In both cases, the output coupler transmission was 13%, but the laser wavelength shifted from 604 nm to 607 nm at higher temperatures.

Vanishing reabsorption in combination with increasing emission cross sections also led to a significant increase of the laser gain at low temperatures. This allows for highly efficient laser operation even at very high output coupler transmissions of up to 60%, which is particularly useful for compact, high-gain amplifier applications.

High gain also decreases the laser threshold inversion, which in turn could increase the threshold doping ion density for the onset of detrimental energy exchange processes between neighboring ions. This may allow for higher doping concentrations, enabling the use of thinner laser crystals, which is beneficial for high-power diode-pumped visible Pr^{3+}-lasers.

This research demonstrates that reducing the operation temperature of orange-emitting Pr^{3+}-lasers – even to moderate levels around 250 K, achievable with thermoelectric cooling – significantly improves their performance. At these temperatures, even oxide materials may enable efficient laser operation. Their typically higher thermal conductivity could contribute to efficient high-power laser operation of Pr^{3+}-lasers at moderately low temperatures.

The research at ZLM thus provides a crucial foundation for optimizing laser crystal compositions and operational temperatures. By exploring practical cooling methods like Peltier elements, the ZLM team aims to make low-temperature laser operation a viable strategy for commercial applications, unlocking new possibilities for high-performance lasers in various applications.

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AlN-Crystal with macroscopic growth steps on N-polar surface *Photo: HORNNISSEN*

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AlN single crystals: Prediction of O-C-Si impurity concentrations from absorption spectra

Aluminium nitride (AlN) single-crystalline wafers have been discussed as possible substrates for a wide range of device applications including ultraviolet light-emitting diodes (UVC-LEDs), UVC laser diodes and lateral power devices. It can be assumed that the commercial use of AlN substrates will only begin after a further increase in diameter to at least 100 mm or more, but also further fundamental studies on point defects are necessary in order to better understand their influence on optical and electrical properties.

The concentrations of the elements oxygen (O), carbon (C) and silicon (Si), which are crucial for absorption and electrical conductivity, are usually measured using secondary ion mass spectrometry (SIMS). As this method is complex and destructive, it would be desirable to derive the concentrations from non-destructive absorption measurements, for example.

In the present work [1], technologies for the intentional introduction of O, C and Si impurities were first developed and then a sample matrix with different impurity concentrations was specifically produced (Fig. 1).

Absorption spectra between 210 nm and 600 nm and chemical concentrations using secondary ion mass spectroscopy (SIMS) were measured on the samples, which were optically polished on both sides and 300 µm thick. The data was used to train a random forest regression tool for deriving impurity concentrations from absorption spectra and the performance of the prediction was tested using so-called "leave one out" tests.

Nominally undoped samples showed [Si] and [C] concentrations in the range $1 \cdot 10^{17}$ - $1 \cdot 10^{18}$ cm^{-3} and [O] concentrations in the range $1 \cdot 10^{18}$ - $1 \cdot 10^{19}$ cm^{-3} and the lowest total impurity concentration of $3 \cdot 10^{18}$ cm^{-3} was achieved with doubly purified source material. The [Si] and [O] concentrations in the source material and the crystals grown with it could be increased to values above $1 \cdot 10^{19}$ cm^{-3} by the addition of Si and O, respectively, in the re-sublimation process of the source material. In contrast, a noticeable increase in the [C] concentrations could only be achieved by the direct addition of carbon in the percentage range to the polycrystalline source in the growth process. It was striking that the [Si] concentrations in the crystals increased to the same extent although the same polycrystalline sources were used in the nominally undoped growths with resulting [Si] concentrations < $1 \cdot 10^{18}$ cm^{-3}.

This behaviour can be explained by theoretical calculations of the formation energies of C_N and Si_{Al} depending on the Fermi energy by Alden et al [2]. With C_N incorporation, the Fermi energy (E_F) is shifted towards the valence band and further C_N incorporation is made more difficult by a then higher C_N formation energy. With Si_{Al} incorporation, E_F is shifted towards the conduction band and further Si_{Al} incorporation is made more difficult by a then higher Si_{Al} formation energy. If C_N and Si_{Al} are incorporated to the same extent, the Fermi energy remains pinned in the centre of the band and the formation energies do not increase.

Samples with high [C] concentrations or a ratio ([O]+[Si])/[C] < 3.3 show peaks or shoulders at a wavelength of 265 nm, which can be attributed to an increase of V_N vacancies caused by an excess of carbon in the crystals. At low [C] content, a low absorption shoulder is formed at 265 nm, which turns into a clearly pronounced maximum with increasing [C] content and finally into a high shoulder.

For Si-dominated samples, the absorption increases in the entire wavelength range with the [Si] concentrations and the absorption spectra exhibit comparatively smooth curves, while [O]-dominated samples show characteristic peaks at 450 nm, but their characteristics do not correlate with the oxygen concentrations. In contrast, there is a clear correlation between the total impurity concentration and the absorption at 230 nm for Si and O-dominated samples.

For so-called "leave one out" tests, a random forest regression tool was trained with 36 SIMS and absorption data sets and then a prediction for the impurity contents was derived for the 37th sample not used for training and compared with the measured SIMS values (Fig. 3). For samples with a high C content (Fig. 3-C), the impurity concentrations and in particular the ratios ([O]+[Si])/[C] were generally well predicted. For Si- and O-dominated samples, the impurity contents were also well predicted, but the differences between [Si] and [O] concentrations were generally predicted slightly lower than measured (Fig. 3: Si-O1-O2). The latter is probably due to the fact that the algorithm cannot distinguish well between the absorption spectra of Si and O-rich samples. As expected, the largest deviations in the predictions were found for samples without neighbouring samples with similar impurity concentrations.

With the sample set of 37 monocrystalline AlN wafers with different impurity concentrations produced within the project framework, it could be shown that a simple random forest regressor model has the potential to derive concentrations of the optically active impurities O, C and Si from absorption spectra, but significantly more samples are required for more precise predictions. An improvement of the prediction accuracy could also be achieved by applying more complex prediction algorithms, which consider the curve shape or shoulders and local maxima as additional information.

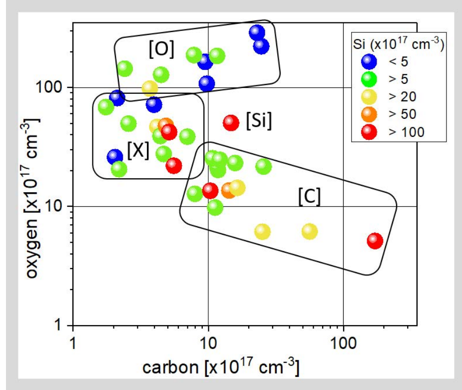

Fig. 1 AlN sample matrix with different O, C and Si impurity concentrations, measured with SIMS - individual areas are indicated with [X] for undoped/silicon doped, with [O] for oxygen doped and with [C] for carbon doped.

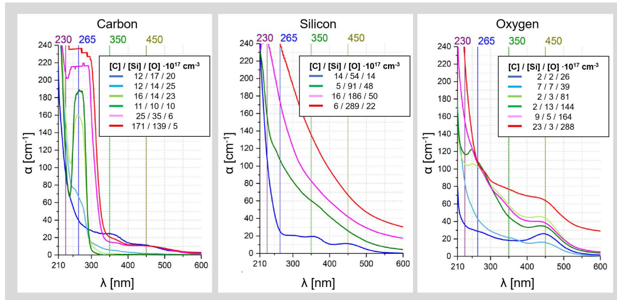

Fig. 2 Typical absorption spectra for samples with ([O]+[Si])/[C] < 3.3 (left), [Si]-dominated samples (centre) and [O]-dominated samples (right).

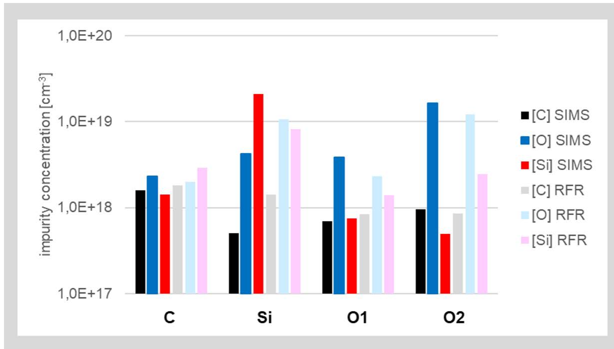

Fig. 3 Impurity concentrations of selected monocrystalline AlN samples measured by secondary ion mass spectroscopy (SIMS) and predicted using a random forest regression tool trained by SIMS values and absorption spectra of 36 training-samples.

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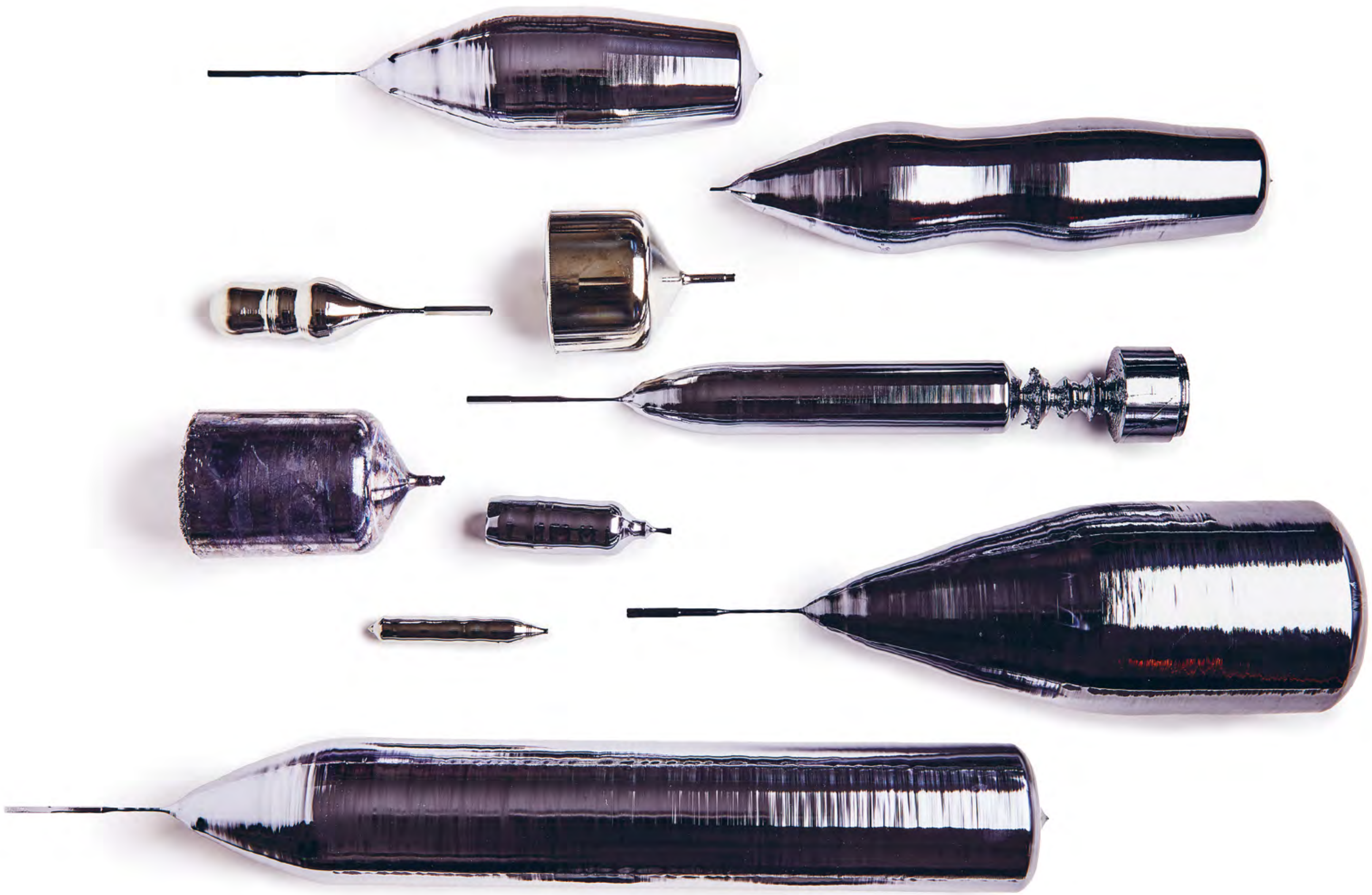

Appendix

Publications
Talks and presentations
Patents
Memberships in committees
Teaching and education

Publications

R. Ahrling, R. Mitdank, A. Popp, J. Rehm, A. Akhtar, Z. Galazka and S. F. Fischer; Resistive and ballistic phonon transport in β-Ga_2O_3; Physical Review B 110 (8) (2024). https://doi.org/10.1103/PhysRevB.110.085302

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M. Zupancic, W. Aggoune, A. Gloter, G. Hoffmann, F. P. Schmidt, Z. Galazka, D. Pfützenreuter, A. A. Riaz, C. Schlueter, H. Amari, A. Regoutz, J. Schwarzkopf, T. Lunkenbein, O. Bierwagen, C. Draxl and M. Albrecht; Polar discontinuity governs surface segregation and interface termination: A case study of $LaInO_3/BaSnO_3$; Physical Review Materials 8 (3) (2024). https://doi.org/10.1103/PhysRevMaterials.8.034602

Talks and presentations

M. Albrecht	C Liu, W. Aggoune, M. Abdeldayem, A. Meldedin, C. Yip, I.-A. Shah,T. Remmele, Y. Sun, Z. Zhang, Y. Yang, A. Fiedler, J. Schwarzkopf, M. Scheffler, D. Zhou	Defect Induced Memristive Switching in off-stoichiometric $SrTiO_3$ and $CaTiO_3$ studied by In Situ Transmission Electron Microscopy	MRS Spring Meeting, 22.-26.04.2024, Seattle, USA
M. Albrecht	M Zupancic , W. Aggoune, A. Gloter, A. Meledin, G. Hoffmann, F.-P. Schmidt, Z. Galazka, D. Pfützenreuter, A. A. Riaz, C. Schlueter, A. Regoutz, J.Schwarzkopf, T. Lunkenbein, O. Bierwagen, Claudia Draxl	The Influence of a Polar-Nonpolar Interfaces on Surface Segregation and Interface Termination: The Case of $LaInO_3/BaSnO_3$	MRS Spring Meeting, 22.-26.04.2024, Seattle, USA
M. Albrecht	C. Wouters, M. Nofal, Piero Mazzolini, J. Zhang, T. Remmele, A. Kwasniewski, O. Bierwagen	Unraveling the atomic mechanism of the disorder–order phase transition from γ-Ga_2O_3 to β-Ga_2O_3	MRS Spring Meeting, 22.-26.04.2024, Seattle, USA
M. Albrecht	M.-H. Lee, R. Schewski, J. B. Varley, T. Remmele, R. L. Peterson	Quantitative Study of Ga Interstitial Diffusion in β-Ga_2O_3: Insights from In Situ Transmission Electron Microscopy and First-Principles Calculations	IWGO5, 27-31.05.2024, Berlin, Germany
M. Albrecht	C. Wouters, M. Nofal, P. Mazzolini, J. Zhang, T. Remmele, A. Kwasniewski, O. Bierwagen, D. Zhou	Unraveling the atomic mechanism of the disorder–order phase transition from γ-Ga_2O_3 to β-Ga_2O_3	IWGO5 2, 27-31.05.2024, Berlin, Germany
M. Badtke	S. Kalusniak, S. Püschel, H. Tanaka, C. Kränkel	Low-doped Tb:YLF for direct blue laser	The 13th Advanced Lasers and Photon Sources Conference (ALPS2024), 22-26.04.2024, Yokohama, Japan
M. Badtke	S. Kalusniak, S. Püschel, H. Tanaka, C. Kränkel	Temperature-dependent performance of yellow and red $Tb^{3+}:LiYF_4$ lasers	13th German-French Workshop on Oxides, Dielectrics, and Laser Crystals (WODIL 2024) 18-19.09.2024, Grenoble, France
M. Badtke	S. Kalusniak, S. Püschel, H. Tanaka, C. Kränkel	Yellow solid-state laser with 61% slope efficiency	Advanced Solid-State Lasers Conference 2024 20-24 .10.2024, Osaka, Japan
M. Bickermann	C. Hartmann	AlN Substrates for UV and Power Applications	5th IKZ Winter School, 28.02-01.03.2024, Berlin, Germany
M. Bickermann	S. Püschel, C. Kränkel, H. Tanaka	Co-doping Effects on Anti-Stokes Fluorescence Cooling in Yb:YLF	54. Deutsche Kristallzüchtungstagung DKT 2024, 6.-8.03.2024, Erlangen, Germany
M. Bickermann	C. Rhode, J. Schreuer, M. Münchhalfen, D. Schlom, Y. E. Li, R. Koc, R. Blukis, C. Guguschev	Growth and Investigation of Hexagallate Substrate Crystals for Strain-engineered Functional Oxide layers	8. European Conference on Crystal Growth (ECCG-8), 21-25.07. 2024, Warsaw, Poland
M. Bickermann	S. Püschel, C. Kränkel, H. Tanaka	Co-doping Effects on Anti-Stokes Fluorescence Cooling in Yb:YLF	8. European Conference on Crystal Growth (ECCG-8), 21-25.07. 2024, Warsaw, Poland
M. Bickermann		Techniques and Applications of Bulk Crystal Growth from the Melt and from Solution	Lecture at the Seminar at the University of Chemical Technology of Prague (VŠChT), 29.08.2024, Prague, Czech Republic

M. Bickermann	Z. Galazka, S. Ganschow, M. Brützam, S. Bin Anooz, T.-S. Chou, A. Popp, T. Straubinger	Bulk Crystals for Novel Semiconductors Prepared at IKZ: Gallium Oxide and Beyond	DGKK workshop on "Bulk Semiconductor Crystals", 09-10.10.2024, Berlin, Germany
M. Bickermann		Growth of Bulk Single Crystals of Novel Semiconductor Materials (AlN, Ga_2O_3, etc.) for Next Generation Efficient Power Electronics	2. International Conference on Materials for Energy & Environmental Engineering (ICM3E 2024), 26-28.11.2024, Algiers, Algeria
I. Buchovska	L. Vieira, F. M. Kiessling, M. Scheffler, J. Klewinghaus, I. Tsiapkinis, R. Menzel	Growth of monocrystalline silicon fibers for mirror suspension in gravitational-wave detectors	GRAvitational - wave Science & technology Symposia (GRASS), 30.09.24-02.10.24, Trento, Italy
I. Buchovska	M. Scheffler, F. M. Kiessling, K. Schindler, L. Vieira, R. Menzel	Growth of monocrystalline silicon fibers for mirror suspension in Einstein Telescope	3rd Einstein Telescope Annual meeting, 12-14.11.24, Warsaw, Poland
I. Buchovska	M. Scheffler, F. M. Kiessling, K. Schindler, L. Vieria, R. Menzel	Monocrystalline silicon fibers developed at IKZ for mirror suspension in Einstein Telescope	Materials for Advanced Detectors 2024 (MAD24), 15.11.24, Warsaw, Poland
K. Dadzis		Multi-physical modeling of bulk crystal growth: from furnace design to defect engineering	20th Conference on Gettering and Defect Engineering in Semiconductor Technology (GADEST 2024), 8-13.09.2024, Bad Schandau, Germany
K. Dadzis		From the growth furnace to a validated virtual model	1st International School on Modelling in Crystal Growth (ISMCG-1), 19-21.09.2024, Timisoara, Romania
K. Dadzis	A. Wintzer, I. Tsiapkinis	New validated open-source models for multi physical simulation of bulk crystal growth	11th International Workshop on Modeling in Crystal Growth (IWMCG-11), 22–25.09.2024, Timisoara, Romania
N. Dropka	M. Holena	Smart furnace and process design for high quality Cz-Si growth at different scales	12th International Workshop on Crystalline Silicon for Solar Cells, 29-31.05.2024, Hangzhou, China
N. Dropka	M. Petkovic, M.Holena	Unraveling Interface Shape and v/G Ratios in Czochralski Growth of Si, Ge, and GaAs through Symbolic Regression	IWMCG-11 22-25.09.2024. Timișoara, Rumänien
N. Dropka	M. Petkovic, X. Tang, G. K. Chappa, L. Vieira, K. Meshram, K. Böttcher, M. Holena	Data driven modelling of bulk crystal growth processes	CRISTECH 2024, 16-18.2024, Angers, France
K. Eremeev	P. Loiko, C. Kränkel, P. Camy, and A. Braud	Excited-state absorption of Tm^{3+}-ions in cubic sesquioxides	Optique Normandie 2025, 01-05 07 2024, Rouen, France
S. Foroushani	K. Dadzis	A modular, low-cost setup for teaching the multiphysics of crystal growth	53. Deutsche Kristallzüchtungstagung (DKT2024), 06-08.03.2024, Erlangen, Germany
C. Frank-Rotsch		Semiconductor bulk crystal growth by vertical gradient freeze (VGF) method	4th European School on Crystal Growth, 17-21.07.2024, Jachranka, Poland
C. Frank-Rotsch		"Semiconductor single crystal growth and the demand for the availability of special metals in the process"	GDMB Expert Committee Special Metals 2024, 18-19.09.2024, Hanau, Germany

Z. Galazka		Bulk crystals and films of β-Ga_2O_3: growth methods and current status	5th IKZ Winter School, 28.02–01.03.2024, Berlin, Germany
Z. Galazka		Bulk rutile-GeO_2 single crystals with extraordinary physical properties	IWGO-5, 26-31.05.2024, Berlin, Germany
Z. Galazka		Bulk Crystal Growth and Physical Properties of Transparent Semiconducting Oxides	ESCG 4, 17-21.07.2024, Jachranka, Poland
Z. Galazka		Bulk single crystals and physical properties of $BaSnO_3$ and $LaInO_3$	German-Korean Workshop, 20-22.08.2024, Berlin, Germany
Z. Galazka		Ultra-Wide Bandgap β-Ga_2O_3 and β-$(Al_xGa_{1-x})_2O_3$ Single Crystals and Their Physical Properties	APWS, 13-17.10.2024, Busan, South Korea
C. Guguschev	C. Guguschev, C. Richter, R. Blukis, T. Remmele, M. Brützam, R. Koc, A. Dittmar, J. Köpp, M. Schulze, S. Ganschow, M. Bickermann, D. G. Schlom	Czochralski growth and characterization of perovskite-type $(Nd,Sr)(Al,Ta)O_3$ single crystals	8th EUROPEAN CONFERENCE ON CRYSTAL GROWTH (ECCG-8), 23.07.2024, Warsaw, Poland
C. Guguschev	C. Guguschev, M. Brützam, R. Koc, M. Schulze, R. Blukis, C. Rhode, C. Richter, J. Köpp, D. Schlom, M. Bickermann	Bulk growth of oxide single crystals using the Czochralski (Cz), top-seeded solution growth (TSSG) and edge-defined film-fed growth (EFG) techniques	Workshop on Tips and Tricks for the Crystal Growth of Inorganic Materials, 26.08.2024, Villingen, Switzerland
C. Kränkel	M. Badtke, S. Kalusniak, S. Püschel, H. Tanaka	Concentration-dependent spectroscopic properties of Tb^{3+}-doped $LiYF_4$ for improved visible diode-pumped solid-state lasers	10th International Workshop on Photoluminescence in Rare Earths: Photonic Materials and Devices, 13.-15.05.2024, Trento, Italy
C. Kränkel	S. Kalusniak, C. Guguschev, R. Koc, D. Schlom	Efficient long wavelength laser operation and spectroscopic characterization of Yb:$LaLuO_3$	Advanced Solid-State Lasers Conference 2024, 20-24 .10.2024, Osaka, Japan
C. Kränkel	S. Kalusniak, M. Badtke, S. Püschel, H. Tanaka	Efficient cryogenic orange Pr:YLF lasers	Advanced Solid-State Lasers Conference 2024, 20-24.10.2024, Osaka, Japan
C. Kränkel	M. Badtke, S. Kalusniak, S. Püschel, H. Tanaka	Yellow solid-state laser with 61% slope efficiency	Advanced Solid-State Lasers Conference 2024, 20-24 10.2024, Osaka, Japan
Z. Liestmann	S. Püschel, S. Kalusniak, C. Kränkel, H. Tanaka	Impact of foreign rare-earth impurities on optical refrigeration of Yb:YLF	SPIE Photonics West 2024, 30.01.-01.02.2024, San Francisco, USA
J. Martin		Dislocations as embedded 1D-nanostructure: Controlling dislocations in epitaxial and stacked heterostructures	Nano2024, 01.07.2024, Lublin, Poland
J. Martin		Update on layer transfer processes of 2D-vdW and twisted perovskites	DGKK wokrshop "Growth Kinetics and Layer Transfer of Ultrathin Layers and 2D Materials", 17.09.2024, Aachen, Germany
P. C. Palleti	A. Gybin, U. Juda, A. Fiedler, N. Schüler, R. Radhakrishnan Sumathi	Investigation of defects affecting minority carrier lifetime in HPGe	German Crystal Growth Association Annual Meeting (DGKK DKT-2024), 06-08.03.2024, Erlangen, Germany

P. C. Palleti	A. Gybin, U. Juda, P. Seyidov, A. Fiedler, N. Schüler, R. Radhakrishnan Sumathi	Investigation of defects influencing the mobility and carrier lifetime in high purity germanium single crystals for radiation detector applications	European Conference on Crystal Growth (ECCG8), 21-25.07.2024, Warsaw, Poland
M. Petkovic		Automating Multi-Objective Optimization with AI	FAIR Automation and AI 13.03.2025, Berlin Berlin, Germany
M. Petkovic	N. Dropka	Leveraging Mathematical Optimization and Machine Learning for Enhanced Numerical Simulations and Process Optimization in Crystal Growth	NUS-ISM-ZIB-IIR-MODAL Workshop on Next Generation Computing and Algorithms in the Digital Era NUS, 12-16.08.2024, Singapore
M. Petkovic		From Energy Systems to Material Science: Optimization as a Common Denominator for a Sustainable Future	Computational Optimization at Work Zuse Institute, 25.09.2024, Berlin, Germany,
M. Petkovic	N. Dropka	SyMO: A hybrid approach for multi-objective optimisation of crystal growth processes	Adlershofer Reserch Forum 11.11.2024, Berlin, Germany
M. Petkovic	N. Dropka, L. Vieira	Smart Data-Driven Approaches for Crystal Growth Process Modeling and Optimization	The IOP-HU Early Career Researcher Conference on Energising Materials 2024, 28-29.11.2024, Berlin, Germany
A. Popp	T.-S. Chou, S. Bin Anooz, J. Rehm, A. Akhtar, Z. Galazka, A. Fiedler, P. Seyidov, K.Irmscher, M. Albrecht	Advances of Homoepitaxial growth of β-Ga_2O_3 by MOVPE	International Workshop on Gallium Oxide 2024, 27.-31.05.2024, Berlin, Germany
A. Popp	T.-S. Chou, S. Bin Anooz, R. Grüneberg, J. Rehm, A. Akhtar, Z. Galazka, A. Fiedler, M. Albrecht, J. Schwarzkopf	Epitaxial Growth of β-Ga_2O_3 Layers	Ultra Wide Bandgap Workshop, 02.07.2025, Berlin, Germany
A. Popp	T.-S. Chou, S. Bin Anooz, Z. Galazka, A. Fiedler, T. Straubinger	Gallium OxideThe Next High Power Material for More Efficient Power Electronics?	Tech Connect: Sustainable Energy Future (Berlin Science Week), 05.11.2025, Berlin, Germany
S. Püschel	C. Kränkel, H. Tanaka	The impact of Er/Tm impurities in Yb:YLF on anti-Stokes fluorescence cooling	The 13th Advanced Lasers and Photon Sources Conference (ALPS2024), 22-26.04.2024, Yokohama, Japan
R. Radhakrishnan Sumathi		High purity semiconductor materials for fundamental and technological applications	International Conference on Emerging Semiconductor Materials and Applications (ICESMA), 8-10.03. 2024, Hyderabad, India
R. Radhakrishnan Sumathi		Contribution of Crystal Growth in redefining the fundamental unit – "the kg-mass"	Public Lecture in the Academy of Sciences Chennai (ASC), 20.03.2024, Chennai, India
R. Radhakrishnan Sumathi	P. C. Palleti	Update on HPGe activities at IKZ	LEGEND Collaboration Meeting, 13-17.05.2024, London, UK
R. Radhakrishnan Sumathi		Growth of Ultra-High-Purity Ge Bulk Single Crystals - Challenges and Opportunities	Asian Conference on Crystal Growth (CGCT-9), 24-26.06.2024, Jeju, South Korea
J. Rehm	T.-S. Chou, A. Akhtar, S. Bin-Anooz, A. Fiedler, M. Schmidbauer, Z. Galazka, A. Popp	Step-flow growth and crystallo-graphic tilting in β-$(AlxGa1\text{-}x)2O_3$ thin films grown on (100) off-oriented β-Ga_2O_3 by MOVPE	International Workshop on Gallium Oxide 2024, 27.-31.05.2024, Berlin, Germany
C. Richter		Lab-Based, Quantitative X-ray Diffraction Imaging Using the Rigaku SmartLab Diffractometer	2024 Rigaku Thin Film XRD Forum, 5.09.2024, Neu-Isenburg, Germany

A. Sabanskis	K. Dadzis	3D simulations of thermal stress-es and validation of a dislocation model for oxide and halide crys-tals grown from the melt	11th International Workshop on Modeling in Crystal Growth (IWMCG-11), 22–25.09.2024, Timisoara, Romania
N. Sagias	A. Wintzer, K. Dadzis	Numerical modeling of furnace design and thermal stresses in the crystal for Czochralski growth of oxides and halides	DGKK-Arbeitskreis "Herstellung und Charakterisierung von massiven Halbleiterkristallen", 09–10.10.2024, Berlin, Germany
T. Schröder	Invited talk / online	How new crystalline materials enter the world of science & technology and reach out to improve daily life in society	Online: Poznan University, 05.04.2024, Poznan, Poland
T. Schröder	Plenary lecture	Latest R & D developments on crystal synthesis & applications	ROCAM Conference Series on Advanced Materials, Romanian Academy and Ministry of Research, Innovation and Digitalization, 15-18.07. 2024, Bucharest, Romania
T. Schröder	Plenary lecture / Opening talk	Crystal Research & Development at IKZ: Status & Trends	8^{th} European Conference on Crystal Growth (ECCG-8), 21-25.07.2024, Warsaw, Poland
T. Schröder		Gallium Oxid Material Basis: Kristalle, Wafer und Epitaxie	Kooperations-Seminar: Wide-Bandgap-Leistungshalbleiter: Herstellung und Anwendungen, Fraunhofer IISB, 15.10.2024, Erlangen, Germany
T. Schulz	A. Lachowski, R. Kernke, M. Albrecht	Cathodoluminescence in a scanning electron microscope operated in transmission mode	20^{th} int. conference on defects, recognition imaging and physics in semiconductors (DRIP), Sony Brook, 18-22.08.2024, New York, USA
J. Schwarzkopf			Photonic Lecture im Sonder-forschungsbereich Transregio 142, 15.05.2024, Paderborn, Germany
J. Schwarzkopf	S. Bin Anooz, M. Abdeldayem, M. de Guimaraes, Y. Wang, C. Liu, M. Albrecht, M. Schmidbauer	MOVPE of complex oxide thin films and their modification by lattice strain and off stoichiometry	16^{Th} IKZ Summer School and German-Korean Workshop, 20.-22.8.2024, Berlin, Germany
J. Schwarzkopf	J. Maltitz, M. Schmidbauer, S. Bin Anooz, J. Martin	Phase Transitions in Free-Standing $(K,Na)NbO_3$ Membranes	MRS Fall Meeting 2024, Symposium NM04: Exploring the Properties and Applications of Freestanding Membranes-From 2D to 3D, 01.-06.12.2024, Boston, USA
J. Schwarzkopf	S. Bin Anooz, M. Abdeldayem, C. Liu, M. Albrecht, I. A. Shah, A. Fiedler, D. Braun, L. v. Helden, M. Schmidbauer	MOVPE of complex oxide thin films and their modification by lattice strain and off-stoichiometry	DGKK+DEMBE 2024 Workshop, 11.-13.12.2024, Berlin, Germany
T. Straubinger	C. Hartmann, Z. Galazka, A. Klump, M. Schulze, M. Bickermann, T. Schröder	Growth and preparation of UWBG crystals AlN and Ga_2O_3 for next generation power electronic	53. Deutsche Kristallzüchtungs-tagung 06-08. 03.2024, Erlangen, Germany
T. Straubinger	A. Klump, C. Hartmann, M. Bickermann	Correlation of impurity concentrations and absorption in aluminum nitride bulk crystals	Tagung des DGKK-Arbeitskreises "Massive Halbleiterkristalle 2024, Berlin Photonics Days 2024, 09.-10.10.2024, Berlin, Germany

A. Subramanian	M. Kabukcuoglu, C. Richter, U. Juda, F. Bärwolf, N.V. Abrosimov, R. Radhakrishnan Sumathi	Growth of B-doped germanium crystals as substrates for high mobility p-MOSFETs	German Crystal Growth Association Annual Meeting (DGKK DKT-2024), 6-8.03.2024, Erlangen, Germany
A. Subramanian	Merve Kabukcuoglu, Carsten Richter, U. Juda, N. Abrosimov, R. Radhakrishnan Sumathi	Dislocation analyses in the boron-doped germanium crystals grown under near-equilibrium conditions	Gettering and Defect Engineering in Semiconductor Technology (GADEST), 08-13.09.2024, Bad Schandau, Germany
H. Tanaka	S. Püschel, Z. Liestmann, C. Kränkel	Optical refrigeration of ytterbium-doped fluoride crystals: From YLF to novel host materials	SPIE Photonics West 2024, 30.01.-01.02.2024, San Francisco, USA
H. Tanaka		Growth of Single Crystals for Electronics and Photonics at IKZ	Japan Electronic Materials Society, The 61st Autumn Meeting, 28-29.10.2024, Tsukuba, Japan
I. Tsiapkinis	K. Dadzis	Melt flow measurements in model experiments for crystal growth	12th Annual jDGKK Meeting, 05.03.2024, Erlangen, Germany
I. Tsiapkinis	A. Wintzer, K. Dadzis	Physical and numerical modeling of the Floating-Zone Process	53. Deutsche Kristallzüchtungstagung (DKT2024), 06-08.03.2024, Erlangen, Germany
I. Tsiapkinis	K. Dadzis	Melt flow measurements in model experiments for crystal growth	4th International Workshop on Measuring Techniques for Liquid Metal Flows (MTLM2024), 27-29.05.2024, Dresden, Germany
I. Tsiapkinis	K. Dadzis	Physical and numerical modeling of the Floating Zone process	11th International Workshop on Modeling in Crystal Growth (IWMCG-11), 22–25.09.2024, Timisoara, Romania
D. Zhou		MEMS-based Environmental Transmission Electron Microscopy	yDGE Electron Microscopy Spring School 2024, 03-06.03.2024, Berlin, Germany
D. Zhou		In Situ Gas Phase ETEM Practical Aspects in the Workflows	Microscopy and Microanalysis 2024, 28.07. -01.08.2024, Cleveland, OH, USA
D. Zhou		In Situ TEM of Oxides	16th IKZ Summer School and German-Korean Workshop, 20.-22.8.2024, Berlin, Germany
D. Zhou	C. Wouters, T. Remmele, J. Zhang, W. Chen, O. Bierwagen, M. Albrecht	In Situ TEM Study on Disorder-Order Phase Transformations of Ga_2O_3	17th European Microscopy Congress 2024, 25-30.08.2024, Copenhagen, Denmark
D. Zhou		In Situ TEM on Semiconductor Materials at IKZ	The IOP-HU Early Career Researcher Conference on Energising Materials 2024, 28-29.11.2024, Berlin, Germany
D. Zhou		In Situ TEM on Off-Stoichiometric $Sr_{1-x}Ti_{1+y}O_3$ and Ga_2O_3	Seminar talk of Department of Semiconductor Physics 04.12.2024, Leipzig, Germany

Patents

Semiconductors

J. Boschker, Ch. Frank-Rotsch, M. Zorn, T. Schröder	Apparatus and method for producing crystals from electrically conductive melts	DE102020131850, US 18/039668
K. Stolze, P. Steglich, K, Berger, U. Juda, J. Martin	Transfer Printable Single-Crystalline Coupons	DE 102022100661.1, EP23151074.4
M. Wünscher, H. Riemann	Apparatus for continuous zone-melting a crystalline rod	DE102012022965B4, EP 2920342B1 (DE, DK, LV)
N. Abrosimov, J. Fischer, H. Riemann, M. Renner	Process and apparatus for producing semiconductor single crystals	DE102010005520B4
D. Souptel, D. Sokolov, Ch. Frank-Rotsch, A. Pötzsch, B. Weinert, O. Root, L. Smejkalova	Improved doped InP crystals	DE102024202321, PCT/EP2025/053419

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Oxides and laser materials

Z. Galazka, R. Uecker, D. Klimm, M. Bickermann	Method for growing beta phase of gallium oxide (ß-Ga_2O_3) single crystals from the melt contained within a metal crucible	EP3242965B1 (AT, BE, CH, DE, CZ, ES, FR, GB, IT, NL, PL), KR101979130B1, US20170362738A1
Z. Galazka, R. Uecker, R. Fornari	Method and apparatus for growing indium oxide (In_2O_3) single crystals and indium oxide (In_2O_3) single crystal	US10208399
C. Guguschev, M. Brützam, D. Schlom, H. Paik	Method and setup for growing bulk single crystals	DE102020114524A1, US20200378030A1, KR1020200138082A
C. Guguschev, E. Haurat, D. Klimm, C. Kränkel, A. Uvarova	Method and device for growing a rare earth sesquioxide crystal	DE102020120715, WO/EP21748512.7
S. Ganschow, C. Kränkel	Method for producing an oxide crystal having a perovskite structure	DE102021134215.3
Z. Galazka, S. Ganschow, M. Bickermann, T. Schröder, W. Häckl	Method and apparatus for producing electrically conducting bulk ß-Ga_20_3 single crystals and electrically conducting bulk ß-Ga_20_3 single crystal	EP22154305.1, PCT/EP/2023051212, TW 112102595
Z. Galazka, S. Ganschow, M. Bickermann, T. Schröder	Melt-grown bulk β-$(Al_xGa_{1-x})_2O_3$ single crystals and method for producing bulk β-$(Al_xGa_{1-x})_2O_3$ single crystals	PCT/EP2022/078252, TW 112138623

Aluminium nitride

A. Dittmar, C. Hartmann, J. Wollweber, M. Bickermann	(Sc,Y):AlN single crystals for lattice-adapted AlGaN systems	KR1020180048926A
C. Hartmann, T. Straubinger	Crystal growth design and method for growing a semiconductor	DE 102022119343.8, US18/363366

Semiconducting layers and nanostructures

O. Ernst, T. Boeck, F. Lange, H.-P. Schramm, T. Teubner, D. Uebel	Method for Microstructuring	DE102020126553
D. Uebel, R. Bansen, T. Boeck, O. Ernst, H.-P. Schramm, T. Teubner	Silicon-based wafers and method of fabricating silicon-based wafers	DE102020132900
O. Ernst, D. Uebel, T. Boeck	Process for the preparation of isotope-enriched germanium-hydrogen compounds	DE 102022105177.3, PCT/EP2023/054384
S. Zahedi-Azad, T. Boeck, O. Ernst, H.-P. Schramm, D. Uebel	Method and growth setup for the fabrication of localized structures	DE 102022116962.6

Oxide layers

M. Albrecht, A. Baki, K. Irmscher, T. Schulz, J. Schwarzkopf, J. Stöver	Formingless Resistive Switching by Off-Stoichiometry Control of ABO_3 Perovskites	DE1020132049, PCT/EP2021/082505
T. Chou, A. Popp, W. Häcklr	Method for producing a gallium oxide layer on a substrate	EP 21187231.2, PCT/EP 2022/069433, TW 111126459
S. Bin-Anooz, T.-S. Chou, W. Häckl, A. Popp	Method for producing a gallium oxide layer on a substrate	EP 22194558.7

X-ray optics

P. Gaal	Providing a transient grid	DE102019132393B4

Memberships in committees

Committees

C. Frank-Rotsch	Secretary of German Association of Crystal Growth (DGKK) German representative of the European Network of Crystal Growth (ENCG) Executive Committee of International Organization for Crystal Growth (IOCG)
C. Guguschev	Commission on Crystal Growth and Characterization of Materials
M. Bickermann	Speaker of the DGKK workgroup "Crystals for Photonics" Elected member of DFG Review Board 405/406 (until April 2024)
R. Radhakrishnan Sumathi	Promosionskommison von Kristian Bader, Fakultät für Geowissenschaften LMU, München
T. Schröder	Deputy Chairman of the "Deutsche Gesellschaft für Kristallzüchtung" DGKK, from Jan 2021 Speaker Leibniz Association: Strategy Forum on Technological Sovereignty; Berlin, 2021 - 2024 Vice-chair of the Leibniz-Section D: Mathematics, Natural Sciences, Engineering of the Leibniz Association, Berlin, since Sep. 2023 Member of the Leibniz Association Presidency in the role of Vice-chair of the Leibniz-Section D, Berlin, since Sep. 2023 Member of Director Nomination Boards of different Leibniz Research Centers, 2024 Coordinator of the European Networks on Crystal Growth (ENCG), Member of council 2022 Member of DESY Photon Science Council, Hamburg, since 2019

Conferences

C. Kränkel	Program Commitee EOSAM European Optical Society Annual Meeting – TOM-07 Ultrafast Phenomena Program Committee Materials Chair Advanced Solid-State Lasers Conference
J. Schwarzkopf	Organizing committee of Material Science and Engineering (MSE) 2024, Symp. F06, Darmstadt
M. Albrecht	15th International Conference on Nitride Semiconductors (ICNS-15), 2024, Oahu, Hawaii, USA: program committee 12th International Workshop on Nitride Semiconductors (IWN) 2024, O'ahu, Hawaii: program committee International Workshop on Gallium Oxide and Related Materials (IWGO) 2024, Berlin: Co-chair
M. Bickermann	8. European Conference on Crystal Growth (ECCG-8) Warsaw, Poland, Member of the International Advisory Committee DGKK workshop on "Bulk Semiconductor Crystals" Berlin-Adlershof, Conference chair and chief organizer International Workshop on Nitride Semiconductors 2024 (IWN 2024) Oahu, Hawaii, USA, Member of the Topical Program Committee Bulk Growth Sessions German-French Workshop on Oxide, Dielectric, and Laser Crystals (WODIL) 2024, Grenoble: Co-Organiser Defects-Recognition, Imaging and Physics in Semiconductors (DRIP) 2024, Stony Brook, NY, USA: Member of the International Steering Committee
K. Stolze	Co-organizer, EMRS Fall Meeting 2024, Symposium H, Warsaw, Poland, Sep 16–19, 2024 Session Organizer "Crystals and films for Detectors", European Conference on Crystal Growth (ECCG-8), Warsaw, Poland International Program Committee Member, Gettering and Defect Engineering in Semiconductor Technology (GADEST)

Journals/editors

M. Bickermann	Editor of the Journal of Crystal Growth (Elsevier B.V.) Associate Editor of the Journal Progress in Crystal Growth and Characterization of Materials (Elsevier B.V.)
N. Dropka	Editor of the Journal Journal of Crystal Growth (Elsevier B.V.)

Teaching and education

M. Bickermann	Crystal Growth I – Fundamentals and Methods	Technische Universität Berlin, Institute of Chemistry
M. Bickermann	Crystal Growth II – Methods and Applications	Technische Universität Berlin, Institute of Chemistry
F. Kießling	Experiments and measurements on crystal growth and crystal structures	Student crystallography laboratory at Lise-Meitner-Schule Berlin
C. Kränkel, T. Schröder (HU Berlin)	Applied Photonics	Humboldt-Universität zu Berlin, Department of Physics
M. Schmidbauer	X-Ray Scattering: Basics and Applications in Materials Science	Humboldt-Universität zu Berlin, Department of Physics
T. Schröder, T. Masselink (HU Berlin), R. Engel-Herbert (PDI)	New directions in electronics, optoelectronics and devices	Humboldt-Universität zu Berlin, Department of Physics
T. Schröder, R. Radhakrishnan Sumathi, J. Martin	Grundlagen und Methoden der modernen Kristallzüchtung – Basics and methods of modern crystal growth	Humboldt-Universität zu Berlin, Department of Physics

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