Annual Report

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

2021

ikz

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Preface

Liebe Leserinnen und Leser,

das Jahr 2021 war wohl eines der erfolgreichsten Jahre in der Geschichte unseres Instituts: Im Oktober 2021 bewilligte die Gemeinsame Wissenschaftskonferenz den kleinen strategischen Sondertatbestand „Kristalltechnologie für Techniksouveränität“ des IKZ. Die zusätzliche Förderung von Bund und Land ab dem Jahr 2023 von 2,2 Mio. € / p. J. ermöglicht es uns, unsere erweiterte IKZ-Strategie „Innovationen in & durch kristalline Materialien“ professionell umzusetzen. Dieser neue IKZ-Strategie-Schwerpunkt ist ein starkes Bekenntnis *unseres Instituts, nicht nur hervorragend in der Wissenschaft zu sein, sondern auch den Technologietransfer im Bereich der kristallinen Materialien zu befördern. Ich bin überzeugt, dass von dieser gestärkten „EU-Flaggschiffrolle“ unseres Institutes im Bereich der Forschung und Entwicklung kristalliner Materialien alle unsere nationalen und internationalen Kooperationen erheblich profitieren werden. Um unsere Position auf dem Gebiet der Materialwissenschaften für die Technologiesouveränität weiter zu stärken, hat das IKZ die Federführung im interdisziplinären Leibniz-Strategieforum „Technologiesouveränität“ übernommen. Gemeinsam mit rund zwanzig weiteren Leibniz-Instituten ist es unser Ziel, die Rolle und Position der Leibniz-Gemeinschaft in diesem wichtigen Politikfeld im kommenden Jahrzehnt zu stärken. Zu diesem Zweck soll das Forum einerseits intern die Kooperationen der verschiedenen Leibniz-Institute in wichtigen Schlüsseltechnologien koordinieren und andererseits als Kontaktplattform zu externen Partnern (besondere aus Politik & Industrie) fungieren. Die Wertschöpfungskette der Schlüsseltechnologien erfordert das konzertierte Handeln vieler Partner, um einen gewissen Grad an Technologiehoheit zu erreichen; die Leibniz-Gemeinschaft ist bereit, mit ihrer Expertise in den Natur- und Sozialwissenschaften sowie in den Wirtschaftswissenschaften zu diesem Ziel beizutragen.*

*Das Jahr 2021 war für das IKZ aber nicht nur im Bereich der Finanzierung seiner Zukunftsstrategie erfolgreich, sondern auch bei der Einwerbung von Drittmitteln für anspruchsvolle wissenschaftliche Projekte. Insgesamt konnten wir im Jahr 2021 Drittmittel für die kommenden Jahre in einer Größenordnung von 5 Mio. € einwerben. Darin enthalten sind etwa 3 Mio. € DFG-Mittel, 1 Mio. € Leibniz-Mittel und etwas weniger als 1 Mio. € Industriemittel. Diese neuen wissenschaftlichen Projekte beginnen rechtzeitig vor der anstehenden „heißen Phase“ der zukünftigen IKZ-Evaluierung im Jahr 2025: Unsere F & E-Ergebnisse in den kommenden Jahren 2022 bis 2024 werden von zentraler Bedeutung für unseren zukünftigen Evaluierungserfolg sein. Hier wird derzeit eine neue Generation von Doktorand:innen am IKZ eingestellt und wir haben heute mehr als ~ 25 Promotionsprojekte in unserem Institut laufen. Im Jahr 2021 konnten wir sieben Promotionsvorhaben erfolgreich abschließen, so viele wie nie zuvor am IKZ. Wir freuen uns, dass unsere Doktorand:innen interessante Arbeitsplätze in ganz unterschiedlichen Bereichen finden. Interessanterweise hat sich die Zahl der IKZ-Mitarbeiter*innen inzwischen auf rund 140 erhöht. Dieser Personalzuwachs und unsere Pläne, die Laborinfrastruktur auszubauen, machen das IKZ-Gebäude immer mehr zum begrenzenden Engpass für unsere zukünftige Entwicklung.*

Das IKZ wurde 2019 umstrukturiert und die neue Abteilungs- und Sektionsstruktur etabliert sich mehr und mehr in unserem täglichen Miteinander. Die interdisziplinäre Zusammenarbeit zwischen den verschiedenen Abteilungen und Sektionen ist unser zentrales Alleinstellungsmerkmal, um das IKZ zu einem wettbewerbsfähigen internationalen Akteur in Wissenschaft und Technologie kristalliner Materialien zu machen. Ein gutes Beispiel für unsere interdisziplinäre Arbeit und unser Engagement für den Technologietransfer ist das IKZ-Start-Up „Tailored X-Ray Product (TXP)“, das von der Gruppe Röntgenoptik in unserer neuen Abteilung für Anwendungswissenschaften gegründet wurde. Hier ist unser IKZ-DESY Joint Lab in Hamburg ein wichtiger Inkubator für den Start und die Weiterentwicklung aktiver röntgenoptischer Produkte, die den zukünftigen Bedürfnissen von Synchrotron- und Freie-Elektronen-Laserquellen der nächsten Generation dienen. Der Zugang zu hochqualitativen kristallinen Materialien ist ein klares „must have“ *für den Erfolg unseres Start-Up Unternehmens.*

Gerne können Sie uns in Berlin im IKZ besuchen!

Mit besten Grüßen

Thomas Schröder

Preface

Dear Readers,

2021 was probably among the most successful years in the history of our institute: In October 2021, the Joint Science Conference approved IKZ´s extraordinary item of expenditure “Crystal Technology for Technology Sovereignty”. The additional funding of 2.2 Mio € / p.a. by state & federal government from 2023 onwards will allow us to implement our extended IKZ strategy “innovations in & by crystalline materials” in a professional way. This new IKZ strategy focus is a strong commitment by our institute to promote not only excellence in science but also transfer of technologies in the area of crystalline materials. I am convinced that from this strengthened EU flagship role of IKZ in R & D on crystalline materials, all our national & international collaborations will substantially benefit. To also further promote our position in the field of materials science for technology sovereignty, IKZ took the lead in the interdisciplinary Leibniz Strategy Forum “Technology Sovereignty”. Here, together with about twenty further Leibniz institutes, our goal is to strengthen the role & the position of the Leibniz association in this important field of politics in the coming decade. For this purpose, the Forum aims to internally coordinate on the one hand the collaborations of the different Leibniz-institutes in important key technologies and act on the other hand as contact platform to external partners (in particular from politics & industry). The value-added chain of key technologies requires the concerted action of many partners to achieve a certain degree of technology sovereignty; the Leibniz association is ready to contribute with its expertise in natural & social sciences as well as in economics to this goal.

The year 2021 was however not only successful for IKZ in the field of funding its future strategy but also in acquiring third party funds for ambitious scientific projects. In total, we could sign in 2021 third party funds for the coming years on the scale of 5 Mio €. These contracts include about 3 Mio € DFG funding, 1 Mio € Leibniz funds and a little bit less than 1 Mio € industry funds. These new scientific projects start right in time for the upcoming “hot phase” of the future IKZ evaluation in 2025: Our R & D results in the coming years from 2022 to 2024 will be of central importance for our future evaluation success. Here, a new generation of Phd students is currently hired at IKZ and we are today running more than ~ 25 Phd projects in our institute. In 2021, we could finish seven Phd defences successfully, more than ever before at IKZ. We are happy to witness that our Phd students find interesting jobs in very different areas. Interestingly, IKZ staff increased meanwhile to about 140 persons working at IKZ. This staff number increase plus our plans to ramp up our laboratory infrastructure make the IKZ building in itself more & more the very limiting bottleneck for our future development.

IKZ restructuring took place in 2019 and the new department & section structure is becoming more and more established in our daily interaction. Interdisciplinary in-house collaborations among the various departments & sections are our central “unique selling points” to make IKZ a competitive international player in science & technology of crystalline materials. A nice demonstration of our interdisciplinary work and our commitment to technology transfer is the IKZ Start-Up “Tailored X-Ray Product (TXP)” funded by the X-Ray Optics group in our new Application Science Department. Here, our IKZ-Desy Joint Lab in Hamburg is an important incubator for the start and further development of active X-ray optics products serving future needs of next generation synchrotron & free electron laser sources. Access to high quality crystalline materials is a clear “must have” for the success of this company.

Feel free to come to Berlin and visit us at the institute!

With kind regards,

Thomas Schröder

Content

The Institute

Photo: Sebastian Rost Fotografie

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

Founded 1992
Part of Forschungsverbund Berlin e.V.
Member of the Leibniz Association

Das Leibniz-Institut für Kristallzüchtung (IKZ)

ist ein internationales Kompetenzzentrum für Wissenschaft & Technologie sowie Service & Transfer im Bereich kristalliner Materialien. Das Spektrum der Forschung und Entwicklung reicht dabei von Themen der Grundlagen- und angewandten Forschung bis hin zu vorindustriellen Forschungsaufgaben.

Kristalline Materialien sind technologische Schlüsselkomponenten zur Realisierung von elektronischen und photonischen Lösungen für gesellschaftliche Herausforderungen. Hierzu gehören künstliche Intelligenz (Kommunikation, Sensorik etc.), Energie (erneuerbare Energien, Energiewandlung etc.) und Gesundheit (medizinische Diagnostik, moderne chirurgische Operationsinstumente etc.). Das IKZ erarbeitet Innovationen *in* kristallinen Materialien durch eine kombinierte Expertise im Haus, bestehend aus Anlagenbau, numerischer Simulation und Kristallzüchtung, um so kristalline Materialien höchster Qualität und mit maßgeschneiderten Eigenschaften zu erforschen.

Zusammen mit Partnern aus Instituten mit angegliederten Technologie-Plattformen sowie Industrieunternehmen treibt das Institut künftig auch verstärkt Innovationen *durch* kristalline Materialien voran. Diese umfassen die zuverlässigen Evaluierungen und Bewertungen innovativer kristalliner Prototypen-Materialien für disruptive Technologieansätze.

Arbeitsschwerpunkte des Institutes sind:

- Entwicklung von Züchtungs-, Bearbeitungs- und Charakterisierungsverfahren für Massivkristalle, kristalline Gebilde mit Abmessungen im Mikro- und Nanometerbereich sowie von materialübergreifenden Kristallzüchtungstechnologien
- Bereitstellung von Kristallen mit besonderen Spezifikationen für Forschungs- und Entwicklungszwecke
- Modellierung und Erforschung der Kristallwachstums- und Kristallzüchtungsprozesse
- Experimentelle und theoretische Untersuchungen zum Einfluss von Prozessparametern auf Kristallzüchtungsvorgänge und Kristallqualität
- Erforschung von Verfahren zur Kristallbearbeitung und der dabei ablaufenden Vorgänge

The Leibniz Institute for Crystal Growth

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 in-house 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

- Physikalisch-chemische Charakterisierung kristalliner Festkörper und Entwicklung geeigneter Methoden bis hin zur atomaren Ebene; Aufklärung des Zusammenhangs zwischen Struktur und Eigenschaften kristalliner Materialien

- Entwicklung und Bau von Anlagenkomponenten für die Züchtung, Bearbeitung und Charakterisierung von Kristallen

Die weitere Materialforschung in Richtung Anwendung ermöglicht verstärkt auch Innovationen *durch* kristalline Materialien:

- Kristall-Prototypenforschung zur zuverlässigen Bewertung innovativer, konfektionierter Kristalle für elektronische und photonische Schlüsseltechnologien

- Prototypen-Lieferfähigkeit neuartiger Kristalle bis zur Kleinserie – in der gewünschten Konfektionierung und Spezifikation – zur zuverlässigen Technologie-Forschung und Vorbereitung der Markteinführung

- Entwicklung von Wafering-Prozessen für neue Materialien, Feinbearbeitung optischer Spezialkristalle

Materialien

- Halbleiter mit großem Bandabstand (Oxide, Aluminiumnitrid) für Hochtemperatur-, Leistungs- und Optoelektronik

- Oxidische und fluoridische Kristalle für Lasertechnik, Optik, Sensorik und Akustoelektronik

- Silizium-Kristalle für Mikro- und Leistungselektronik und Photovoltaik

- Isotopenreine Halbleiter (Silizium und Germanium) für die Quantentechnologie

- Silizium/Germanium Kristalle für Strahlungsdetektoren und Beugungsgitter, kristalline Si/Ge-Schichten für thermoelektrische Anwendungen

- Ferroelektrische und halbleitende Oxidschichten für die Mikro- und Leistungselektronik, Sensoren und Datenspeicher

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- 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 photon

- 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

- 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 and photovoltaics

- 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 thermoelectric devices

- Ferroelectric and semiconducting oxide layers for micro- and power electronics, sensor applications or data storage

Das IKZ als familienfreundlicher Arbeitgeber

Das IKZ möchte seinen Beschäftigten ein offenes, kooperatives und familienfreundliches Arbeitsumfeld bieten. Das Institut unterstützt daher seine Mitarbeiterinnen und Mitarbeiter bei der Vereinbarkeit von Arbeit und Familie, z.B. durch flexible Regelungen zur täglichen Arbeitszeit oder durch variable Regelungen zu Teil- und Vollzeitbeschäftigung.
Seit 2015 ist das Institut zertifiziert durch das *audit berufundfamilie*. Damit verbunden hat es Ziele einer familienbewussten Personalpolitik definiert und sich diesen verpflichtet. In den folgenden drei Jahren haben wir die in diesem Prozess definierten Maßnahmen umgesetzt. Die Zertifizierung wurde 2018 und 2021 erneut an das Institut vergeben.

Das Audit steht unter der Schirmherrschaft der Bundesfamilienministerin und des Bundeswirtschaftsministers, nähere Informationen finden sich unter
www.beruf-und-familie.de

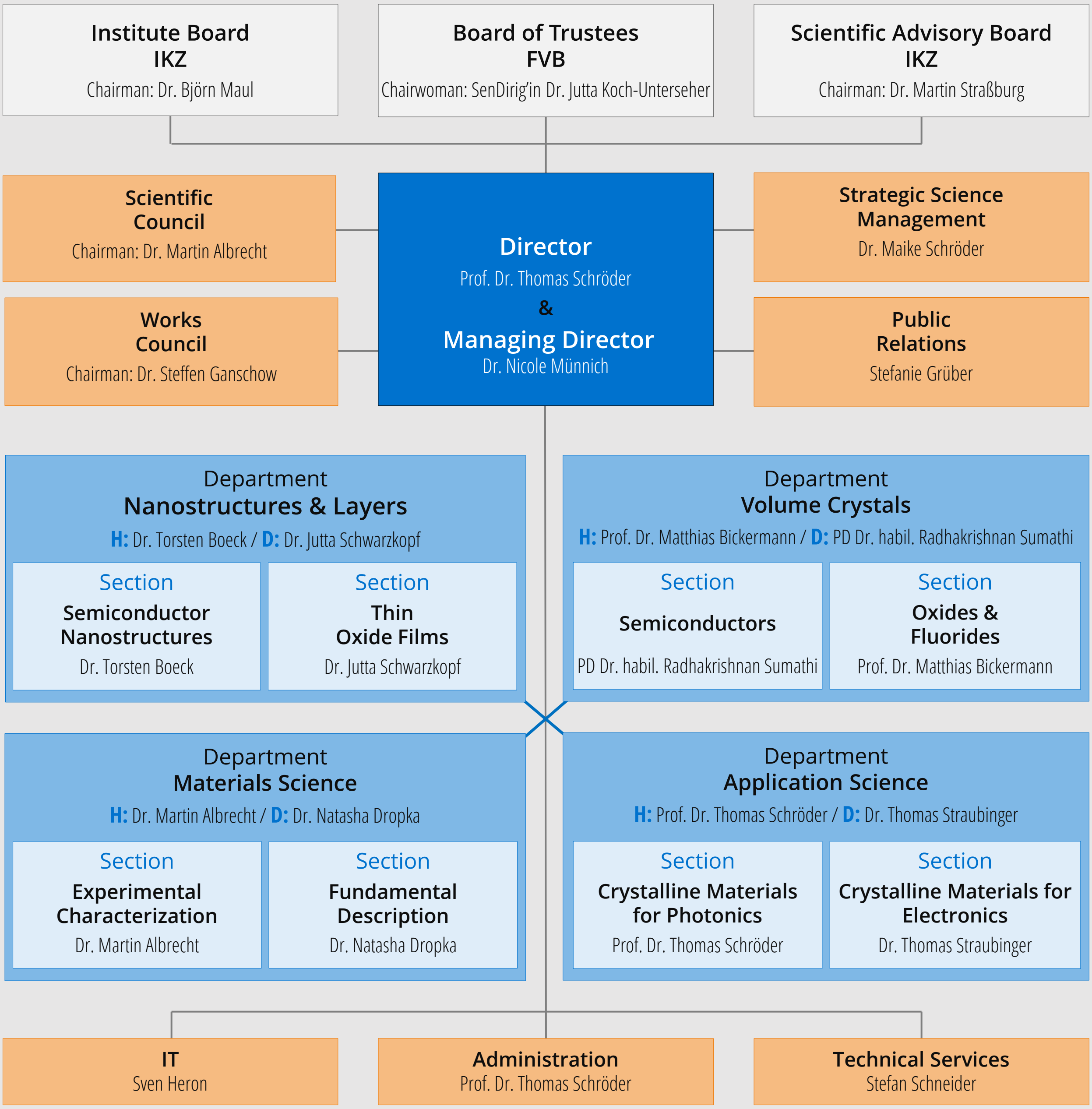
IKZ as family-friendly employer

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 audit has been renewed in 2018 and 2021.

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 wwww.beruf-und-familie.de

Zertifikat seit 2015
audit berufundfamilie

Organigramm 2021
Organisation Chart 2021



Institute Board
IKZ
Chairman: Dr. Björn Maul

Board of Trustees
FVB
Chairwoman: SenDirig'in Dr. Jutta Koch-Unterseher

Scientific Advisory Board
IKZ
Chairman: Dr. Martin Straßburg

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Chairman: Dr. Steffen Ganschow

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Prof. Dr. Thomas Schröder
&
Managing Director
Dr. Nicole Münnich

Strategic Science Management
Dr. Maike Schröder

Public Relations
Stefanie Grüber

Department
Nanostructures & Layers
H: Dr. Torsten Boeck / **D:** Dr. Jutta Schwarzkopf

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Semiconductor Nanostructures
Dr. Torsten Boeck

Section
Thin Oxide Films
Dr. Jutta Schwarzkopf

Department
Volume Crystals
H: Prof. Dr. Matthias Bickermann / **D:** PD Dr. habil. Radhakrishnan Sumathi

Section
Semiconductors
PD Dr. habil. Radhakrishnan Sumathi

Section
Oxides & Fluorides
Prof. Dr. Matthias Bickermann

Department
Materials Science
H: Dr. Martin Albrecht / **D:** Dr. Natasha Dropka

Section
Experimental Characterization
Dr. Martin Albrecht

Section
Fundamental Description
Dr. Natasha Dropka

Department
Application Science
H: Prof. Dr. Thomas Schröder / **D:** Dr. Thomas Straubinger

Section
Crystalline Materials for Photonics
Prof. Dr. Thomas Schröder

Section
Crystalline Materials for Electronics
Dr. Thomas Straubinger

IT
Sven Heron

Administration
Prof. Dr. Thomas Schröder

Technical Services
Stefan Schneider

Wissenschaftlicher Beirat 2021
Scientific Advisory Board 2021

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Regensburg, Germany

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Mikroelektronik
Frankfurt/Oder, Germany

Vertreter des Landes Berlin
Representative of the State of Berlin

Dr. Björn Maul
Referat Natur-, Material- und Lebenswissenschaften
Der Regierende Bürgermeister von Berlin
Senatskanzlei VI D
Berlin, Germany

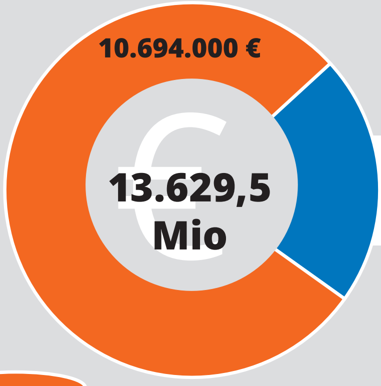
Vertreter der Bundesrepublik Deutschland
Representative of the Federal Republic of Germany

Christoph Schwickart
Bundesministerium für Bildung und Forschung BMBF
Bonn/Berlin, Germany

2021 in Zahlen
2021 in figures

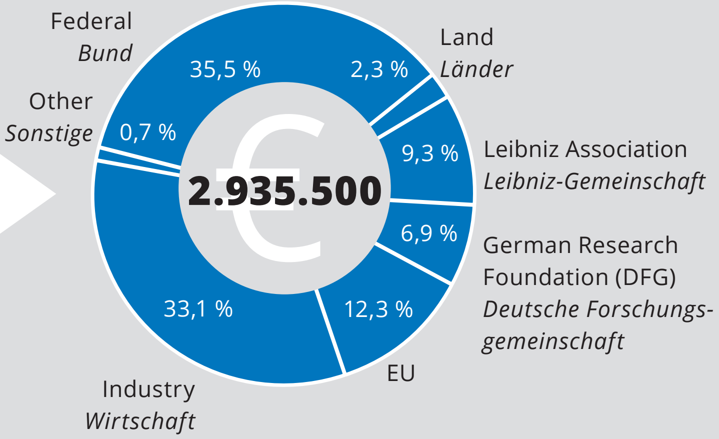
Budget Gesamt
Total

Institutional funding
Institutionelle Förderung



2.935.500 €
Third-party funding
Drittmittelförderung

Drittmittelförderung
Third-party funding



Lehre
Education

7 Defended doctoral theses
Abgeschlossene Promotionsarbeiten

24 Ongoing dissertations
Laufende Promotionsvorhaben

9 Master theses completed
Abgeschlossene Masterarbeiten

Publikationen
Publications

80 Articles in peer-reviewed journals
Artikel in referierten (peer-review) Journalen

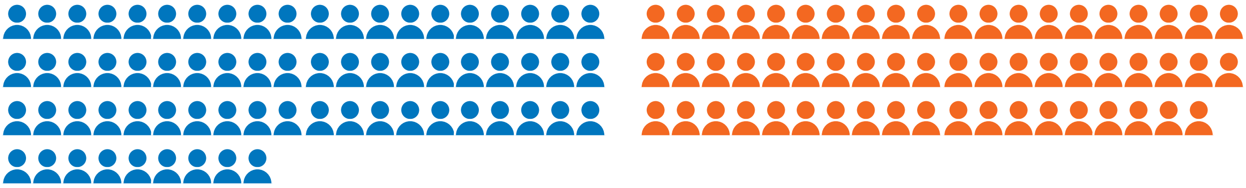
Stichtag 31.12.2021

Internationalisierung
Internationalization

Staff members from 23 countries
Beschäftigte aus 23 Ländern

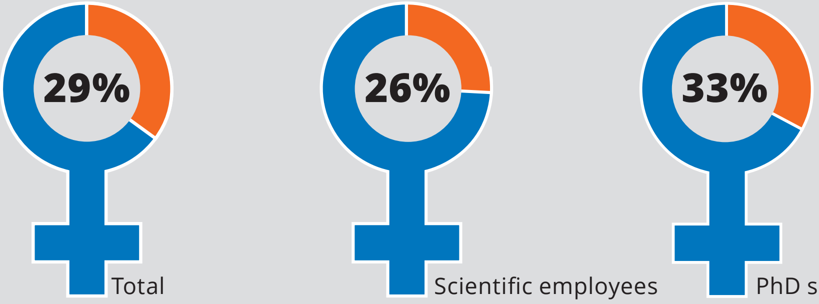
Personal gesamt
Staff total

139



69 Scientific employees
Wissenschaftliche Mitarbeiter/innen

59 Infrastructure personnel
Infrastrukturpersonal



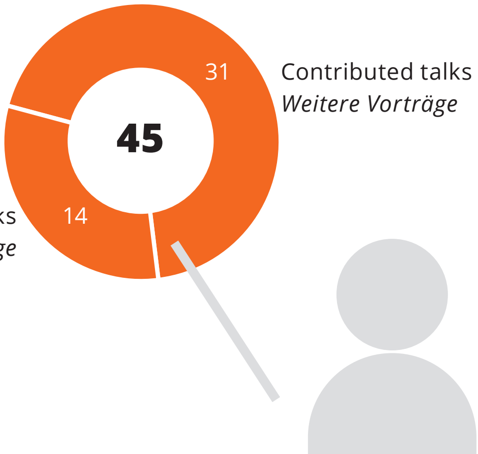
Total
Gesamt

Scientific employees
Wissenschaftliche Mitarbeiterinnen

PhD students
Doktorandinnen

Frauenanteil
Female proportion

Beiträge auf internationalen Konferenzen
Contributions in international conferences



Contributed talks
Weitere Vorträge

Invited talks
Eingeladene Vorträge

Das Leibniz-Strategieforum *Technologische Souveränität*

The Leibniz Strategy Forum *Technological Sovereignty*

Mit der Gründung des Leibniz-Strategieforums (2021) möchte die Leibniz-Gemeinschaft auf Basis des BMBF-Impulspapiers „Technologisch souverän die Zukunft gestalten“ mit ihren Kompetenzen und Instituten einen effektiven Beitrag zur Stärkung der technologischen Souveränität (TS) von Deutschland und Europa leisten.

Die TS Europas hat eine globale Dimension. Sie definiert wesentlich den Anspruch Europas, neben den asiatischen und amerikanischen Werte- und Wirtschaftsmodellen einen ebenbürtigen europäischen Weg zu verfolgen. Dies beinhaltet die Aufgaben:

- weltweit führend in Ausbildung, Forschung und Entwicklung zu sein;
- eine kompetitive Wirtschaftsstruktur im Bereich der Schlüsseltechnologien zu besitzen;
- ein Gesellschaftsmodell mit den Werten europäischer Demokratien zu leben;
- Standards und Normen der weltweiten Handelspolitik bei Zukunftstechnologien mitzugestalten.

Die Notwendigkeit dieser Arbeitsgebiete ergibt sich daraus, dass sich im Bereich der Hochtechnologie zunehmend protektionistische Züge in den Wirtschaftsverhältnissen zwischen Ländern verschiedener gesellschaftlicher Wertesysteme zeigen. Ein Beispiel sind Exportbeschränkungen im Bereich des Zugangs zu modernen Halbleiterchips, die als Schlüsseltechnologie viele Bereiche der Wertschöpfung und Gesellschaft berührt.

Das IKZ übernimmt die Federführung der Organisation des Leibniz-TS-Forums mit Herrn Prof. Thomas Schröder als Sprecher. Aufgabe des TS-Forums ist es, ganzheitliche Beiträge der Leibniz-Institute zu Wertschöpfungsketten in Schlüsseltechnologiefeldern zu erarbeiten und diese mit komplementären Partnern in der Wertschöpfungskette zu vernetzen mit den folgenden Zielen:

By founding the Leibniz Strategy Forum (2021), the Leibniz Association intends to effectively contribute to the strengthening of the Technological Sovereignty (TS) of Germany and Europe with its skills and institutes on the basis of the BMBF‘s impulse paper „Shaping the Future with Technological Sovereignity“.

Europe‘s TS has a global dimension. It essentially defines Europe‘s claim to pursue an equal European way alongside the Asian and American value and economic models. This includes the tasks of

- being a world leader in education, research and development;
- having a competitive economic structure with respect to key technologies;
- living a social model with the European values of democracy;
- shaping standards and norms of global trade policy in future technologies.

The need for these topics arises from the fact that in the field of high technology, protectionist features are increasingly evident in economic relations between countries with different social value systems. One example is export restrictions of modern semiconductor chips, which as a key technology touches many areas of value creation and society.

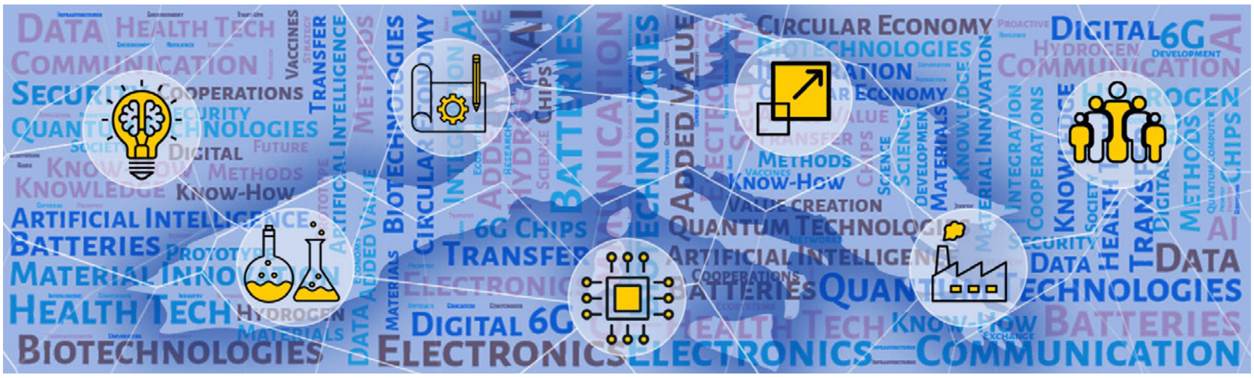
The IKZ takes the lead in organising the Leibniz TS Forum (spokesman: Prof. Thomas Schröder) which has two main tasks: 1) the development of holistic contributions of the Leibniz institutes to value chains in key technology fields and 2) the linkage of Leibniz institutes with complementary partners in the value chain for the:

- Schaffung der Sichtbarkeit der Leibniz-Potentiale in Politik, Gesellschaft und Wirtschaft,
- Bündelung und Ausbau der Potentiale der Leibniz-Gemeinschaft zur Schaffung einer technologischen Hoheit in Deutschland und Europa,
- komplementäre Einordnung und Einbindung in die nationale / europäische Forschung und Wirtschaft, gemeinsam mit anderen außeruniversitären Forschungseinrichtungen (AUFs),
- Erstellung eines Maßnahmenkatalogs / Arbeitsprogramms als Leibniz-Beitrag zur TS Europas.

Sechs Leibniz-Cluster werden aktiv im Leibniz-Forum zu den folgenden gesellschaftlichen Thematiken entwickelt: Gesundheitstechnologien, Künstliche Intelligenz, Materialien für die Digitalisierung, Quantentechnologien, Wasserstoffwirtschaft und Zukunftskommunikation.

- creation of visibility of Leibniz potentials in politics, society and economy,
- focusing and expanding the potentials of the Leibniz Association to create TS in Germany and Europe,
- complementary classification and integration into national / European research and economy by cooperation with other non-university research institutions (AUFs),
- drawing up a catalogue of measures / working programs as Leibniz contribution to the TS of Europe.

Six Leibniz clusters are actively developed in the Leibniz Forum on social topics: Health Technologies, Artificial Intelligence, Materials for Digitalisation, Quantum Technologies, Hydrogen Economy and Future Communication.



Veranstaltungen

Das TS-Forum präsentierte sich 2021 in drei öffentlichen Veranstaltungen: Auf der *Berlin Science Week 2021* in Form einer Podiumsdiskussion und in den Veranstaltungen *Leibniz debattiert* und *Leibniz meets Industry*. Zusätzlich wurde das Forum in der Zeitschrift *Cluster Optik & Photonik* (Interview mit Herrn Prof. Schröder und Herrn Dr. Allahgholi), dem *Leibniz-Magazin* (Interview mit Herrn Prof. Schröder und Frau Prof. Flach) und dem *Adlershof-Journal* (Interview mit Herr Prof. Schröder) vorgestellt.

Die Videoaufzeichnungen der Veranstaltungen sowie die vollständigen Interviews finden Sie unter: **https://www.ikz-berlin.de/ueber-uns/leibniz-strategieforum-technologische-souveraenitaet**

In Bezug auf diese Öffentlichkeitsarbeit soll hier die Podiumsdiskussion auf der *Berlin Science Week 2021* näher vorgestellt werden.

Events

The TS Forum was presented in three public events in 2021: 1) *Berlin Science Week 2021* (panel discussion); 2) *Leibniz debates* and 3) *Leibniz meets Industry*. Further information about the Forum were given in the magazine *Cluster Optik & Photonik* (interview with Prof. Schröder and Dr. Allahgholi), the *Leibniz Magazine* (interview with Prof. Schröder and Prof. Flach) and the *Adlershof Journal* (interview with Prof. Schröder). The video recordings of the events as well as the complete interviews can be found at:

https://www.ikz-berlin.de/ueber-uns/leibniz-strategieforum-technologische-souveraenitaet

With regard to this public work, the panel discussion at *Berlin Science Week 2021* will be presented in more detail.

Berlin Science Week 2021 – Podiumsdiskussion

Eine Schlüsseltechnologie, in der Berlin Vorreiter sein kann, ist die Materialwissenschaft. Sie bietet das große Potential, Vorsprung durch Technologie in bestehenden Märkten zu erarbeiten bzw. gar völlig neuartige, disruptive Technologien zu ermöglichen. Berlin verfügt über eine umfangreiche Expertise im außeruniversitären und universitären Sektor, um die Materialforschung wissenschaftlich und wirtschaftlich voranzutreiben. Aber auch ein politischer Wille ist entscheidend, um zusammen mit Wissenschaft und Wirtschaft Strategien zur TS in der Materialwissenschaft zu erarbeiten. Hier bietet gerade der Standort Adlershof große Potentiale, eine führende Rolle einzunehmen.

Um diese wissenschaftlichen, wirtschaftlichen und politischen Strategien der TS in der Materialwissenschaft von verschiedenen Standpunkten zu beleuchten, standen in der *Berlin Science Week 2021* Expertinnen und Experten aus verschiedenen Bereichen Rede und Antwort:

Berlin Science Week 2021 – Panel Discussion

One key technology in which Berlin could take on a leading position is materials science. It offers great potential to develop an advance through technology in existing markets or even to enable completely new, disruptive technologies. Berlin has extensive expertise in the non-university and university sectors to advanced materials research - scientifically and economically. But political support is also crucial in order to develop strategies for TS in materials science together with science and industry. Here, in particular the Adlershof location offers great potential to take the lead.

To get a closer look at these scientific, economic and political strategies for TS in materials science, experts from various fields were available to answer questions during *Berlin Science Week 2021*:

- **Prof. Thomas Schröder**
  Institut für Kristallzüchtung (IKZ), Moderation
- **Prof. Marcel Fratzscher**
  Deutsches Institut für Wirtschaftsforschung (DIW)
- **Engelbert Beyer**
  Bundesministerium für Bildung und Forschung (BMBF)
- **Dr. Ursula Eul**
  Fraunhofer-Verbund Werkstoffe, Bauteile-Material
- **Prof. Oliver Kraft**
  Karlsruher Institut für Technologie (KIT)
- **Prof. Bernd Rech**
  Helmholtz-Zentrum Berlin (HZB)
- **Dr. Jutta Koch-Unterseher**
  Senatsverwaltung für Bildung, Wissenschaft und Forschung in Berlin
- **Prof. Sabine Kunst**
  Berlin University Alliance (BUA)
  Präsidentin der Humboldt-Universität zu Berlin

Es wurde die Bedeutung von Materialforschung auf europäischen Level aus politischer und wirtschaftlicher Sicht diskutiert. Um wissenschaftlich einschlägig zu handeln, müssen Kräfte gebündelt werden und Partnerschaften zwischen den AUFs untereinander und auch mit den Universitäten etabliert werden. Dies erfordert die Definition von wissenschaftspolitischen Zielen auch auf Berliner Ebene.

- **Prof. Thomas Schröder**
  Leibniz-Institut für Kristallzüchtung (IKZ), moderator
- **Prof. Marcel Fratzscher**
  German Institute for Economic Research (DIW)
- **Engelbert Beyer**
  Federal Ministry of Education and Research (BMBF)
- **Dr. Ursula Eul**
  Fraunhofer Groups
- **Prof. Oliver Kraft**
  Karlsruhe Institute of Technology (KIT)
- **Prof. Bernd Rech**
  Helmholtz-Zentrum Berlin (HZB)
- **Dr. Jutta Koch-Unterseher**
  Senate Administration for Education, Science and Research in Berlin
- **Prof. Sabine Kunst**
  Berlin University Alliance (BUA)
  President of Humboldt-Universität zu Berlin (HUB)

The importance of materials research on a European level from a political and economic point of view was discussed. In order to act in a scientifically relevant way, forces must be focused and partnerships between the AUFs and universities must be established. This requires the definition of science policy goals also at the Berlin level.

Forschungsverbund Berlin mit neuer Geschäftsführerin

Dr. Nicole Münnich hat ab dem 1. Dezember 2021 die Geschäftsführung des Forschungsverbundes Berlin e.V. übernommen. Sie folgt auf Dr. Falk Fabich, der nach dem Weggang der langjährigen Geschäftsführerin seit April 2021 die kommissarische Geschäftsführung innehatte.

Nicole Münnich ist promovierte Historikerin und erfahrene Wissenschaftsmanagerin. Zuvor leitete sie das Referat „Hochschulen, wissenschaftliche Zentren, Digitalisierung und Künstliche Intelligenz" und war Stellvertretende Leiterin der Abteilung Wissenschaft und Forschung im Ministerium für Wissenschaft, Forschung und Kultur des Landes Brandenburg.

„Wir freuen uns sehr, dass wir mit Dr. Nicole Münnich eine versierte Wissenschaftsmanagerin gewinnen konnten. Mit ihrer Expertise werden wir unsere Verbundverwaltung zukunftsorientiert weiterentwickeln", erklärt Prof. Thomas Schröder, Vorstandssprecher des Forschungsverbundes Berlin.

Der FVB ist eine der größten außeruniversitären Forschungseinrichtungen Berlins. Er besteht aus sieben Instituten der Natur-, Ingenieur-, Lebens- und Umweltwissenschaften. Die Institute des Forschungsverbundes Berlin sind Mitglieder der Leibniz-Gemeinschaft und werden gemeinsam durch Bund und Länder finanziert. Der FVB bietet den sieben Instituten eine gemeinsame Verwaltung – so ergeben sich wichtige Synergien in Administration und Governance – sowie eine Plattform für den Austausch von Wissenschaftlerinnen und Wissenschaftlern.

www.fv-berlin.de

Foto: Ralf Günther

Forschungsverbund Berlin with new Managing Director

Dr. Nicole Münnich has taken over as Managing Director of the Forschungsverbund Berlin e.V. (FVB) on December 1, 2021. She succeeds Dr. Falk Fabich, who was Acting Managing Director from April 2021 due to the departure of long-time Managing Director Dr. Manuela Urban.

Nicole Münnich holds a doctorate in history, and is an experienced science manager. Before joining FVB, she headed the "Universities, Scientific Centers, Digitalization, and Artificial Intelligence" unit and was Deputy Head of the Science and Research Department at the Ministry of Science, Research and Culture of the Federal State of Brandenburg.

"We are delighted to have been able to recruit Dr. Nicole Münnich, an experienced science manager. With her expertise, we will continue to develop our Joint Administration in a forward-looking way," stated Professor Thomas Schröder, Executive Board Spokesman of the Forschungsverbund Berlin.

FVB is one of Berlin's largest non-university research institutions. It comprises seven institutes in the fields of natural, engineering, life and environmental sciences. The institutes under the umbrella of the Forschungsverbund Berlin are members of the Leibniz Association, and are funded jointly by the German federation and the federal states. FVB provides its seven institutes with a Joint Administration, creating key synergies in administration and governance, as well as a platform for academic exchange.

www.fv-berlin.de

Thomas Schröder ist neuer Vorstandssprecher des Forschungsverbundes Berlin

Prof. Thomas Schröder ist seit dem 1. September 2021 neuer Vorstandssprecher des Forschungsverbundes Berlin e.V. (FVB). Die Amtszeit beträgt zwei Jahre. Stellvertretender Vorstandssprecher ist Prof. Stefan Eisebitt, Direktor am Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie (MBI).

Als Vorstandssprecher vertritt Thomas Schröder institutsübergreifende gemeinsame und allgemeine Interessen des FVB – und setzt dabei Schwerpunkte. „Digitalisierung, Internationalisierung und Gleichstellung sind Themen, die ich in meiner Zeit als Vorstandssprecher engagiert verfolgen werde. Ein weiteres Ziel ist ein klimaneutraler FVB – diesem Thema müssen wir uns stellen und unsere Gebäude energieeffizient entwickeln. Dies ist ein großes politisches Ziel, das der FVB gemeinsam mit den Zuwendungsgebern Land und Bund angehen muss“, erklärt er.

Thomas Schröder is the new Executive Board Spokesman of Forschungsverbund Berlin

Professor Thomas Schröder, Director of the Leibniz-Institut für Kristallzüchtung (IKZ), is the new Executive Board Spokesman of the Forschungsverbund Berlin e.V. (FVB) as of September 1, 2021. The term of office is two years. Deputy Executive Board Spokesman is Professor Stefan Eisebitt, Director at the Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy (MBI).

As Executive Board Spokesperson, Thomas Schröder represents the common and general interests of FVB across all institutes, setting priorities in the process. “Digitalization, internationalization and equality are issues that I shall vigorously pursue during my time as Executive Board Spokesperson. Another goal is to achieve a climate-neutral FVB – we must address this issue and make our buildings energy-efficient. This is a major political goal that FVB will need to address together with its awarding authorities – the state and federal governments,” he states.

Veranstaltungen
Events

IKZ Sommerschule: Oxides for electronic applications

In Kooperation mit dem Leibniz-WissenschaftsCampus GraFOx fand vom 16. – 18. August 2021 die 13. IKZ Sommerschule statt. Aufgrund der Corona-Pandemie wurde die Veranstaltung zum Thema „Oxides for electronic applications“ online abgehalten. Fast 100 Teilnehmende aus 12 Ländern nahmen die Möglichkeit des 2020 neu etablierten Veranstaltungsformates wahr. Es war die am stärksten besuchte IKZ Schule seit Beginn der Veranstaltungsreihe.

Huili (Grace) Xing und Debdeep Jena von der Cornell University, USA, referierten zur elektronischen Struktur von Oxiden, zu den Grundlagen der Oxidelektronik sowie zum Stand der Technik im Bereich der Ga_2O_3-Elektronik. Neben einer Postersession wurde den Teilnehmern die Möglichkeit zu ausführlicher Diskussion in getrennten digitalen Räumen gegeben.

Huili (Grace) Xing hält eine William L. Quackenbush Professur für Elektrotechnik und Computertechnik an der Cornell Universität. Debdeep Jena ist ein Richard E. Lunquist Sesquicentennial Faculty Fellow und ebenfalls Professor an der Cornell Universität. Gemeinsam betreiben sie das Jena-Xing-Labor zur Entwicklung von Halbleitern für die Elektronik und zum Verständnis fundamentaler Grenzen dieser Materialien und ihrer Anwendungen. Die Arbeiten der Gruppe beruhen auf der Herstellung von Strukturen mittels Epitaxie, grundlegender Materialcharakterisierungen sowie der Transporttheorie.

IKZ summer school: Oxides for electronic applications

The 13th IKZ Summer School on “Oxides for electronic applications” in cooperation with the Leibniz ScienceCampus GraFOx took place from 16 – 18 August 2021. Due to the pandemic, the event was held online, and nearly 100 participants from 12 countries took the opportunity of this new event format established in 2020. It was the most attended IKZ school since the beginning of the event series.

Huili (Grace) Xing and Debdeep Jena from Cornell University, USA, lectured on the electronic structure of oxides, the fundamentals of oxide electronics, and the state of the art in Ga_2O_3 electronics. In addition to a poster session, participants were given the opportunity for extensive discussion in separate digital rooms.

Huili (Grace) Xing holds a William L. Quackenbush Professorship in Electrical and Computer Engineering at Cornell University. Debdeep Jena is a Richard E. Lunquist Sesquicentennial Faculty Fellow and also a professor at Cornell University. Together, they run the Jena-Xing Laboratory to develop semiconductors for electronics and to understand fundamental limitations of these materials and their applications. The group’s work is based on fabrication of structures using epitaxy, fundamental materials characterization, and transport theory.

IKZ Winterschule: Layer Transfer Technologie – From artificial crystals to novel applications

Auch die IKZ Winterschule präsentierte sich in diesem Jahr erneut im Online-Format. Vom 8. – 10. Dezember 2021 verfolgten 63 interessierte WissenschaftlerInnen, Postdocs, Promovierende und Masterstudierende aus 9 Ländern den Ausführungen der Dozenten zum Thema „Layer Transfer“.

Layer Transfer stellt einen Paradigmenwechsel in der Synthese von kristallinen Heterostrukturen dar. Im Gegensatz zu etablierten Wachstumsmethoden für epitaktische Heterostrukturen, bei denen die Bedingungen an der Grenzfläche in Bezug auf Oberflächenenergien, Gitterparameter und Kristallsymmetrie übereinstimmen müssen, erlaubt der Layer Transfer prinzipiell die Kombination beliebiger kristalliner Materialien. Das Potenzial zur Herstellung neuartiger künstlicher kristalliner Heterostrukturen wurde mit 2-dimensionalen van der Waals-Materialien wie Graphen demonstriert. Im Rahmen des Workshops wurden die neuesten Entwicklungen zur Integration von 2D-Materialien und funktionalen Oxiden in die Silizium-Technologie diskutiert. Außerdem wurde eine breite Palette von modernsten Layer Transfer-, Micro Transfer Printing- und Wafer Bonding-Technologien behandelt.

Zu den Dozenten zählten: Dr. Jens Martin (IKZ, Berlin), Prof. Dr. Emil J. W. List-Kratochvil (Humboldt-Universität zu Berlin; Helmholtz Zentrum Berlin), Prof. Dr. Max Lemme (RWTH Aachen University; AMO GmbH, Aachen), Dr. Jean Fompeyrine (Lumiphase AG; Kilchberg, Switzerland), Prof. Dr. Andreas Mai (TH Wildau, Leibniz Institute for High Performance Microelectronics IHP) und Dipl.-Ing. (FH) Kai Zoschke (Fraunhofer Institute for Reliability and Microintegration IZM).

IKZ winter school: Layer Transfer Technologies – From artificial crystals to novel applications

This year, the IKZ Winter School was once again presented in an online format. From December 8-10, 2021, 63 interested scientists, postdocs, PhD and Master students from 9 countries followed the lecturers’ explanations on the topic of "Layer Transfer".

Layer Transfer represents a paradigm shift in the synthesis of crystalline heterostructures. In contrast to established growth methods for epitaxial heterostructures, where the conditions at the interface have to match in terms of surface energies, lattice parameters and crystal symmetry, Layer Transfer in principle allows the combination of arbitrary crystalline materials. The potential to fabricate novel artificial crystalline heterostructures was demonstrated with 2-dimensional van der Waals materials such as graphene. During the workshop, the latest developments on the integration of 2D materials and functional oxides into silicon technology were discussed. A wide range of state-of-the-art layer transfer, micro transfer printing and wafer bonding technologies were also covered.

The lecturers were: Dr. Jens Martin (IKZ, Berlin), Prof. Dr. Emil J. W. List-Kratochvil (Humboldt-Universität zu Berlin; Helmholtz Zentrum Berlin), Prof. Dr. Max Lemme (RWTH Aachen University; AMO GmbH, Aachen), Dr. Jean Fompeyrine (Lumiphase AG; Kilchberg, Switzerland), Prof. Dr. Andreas Mai (TH Wildau, Leibniz Institute for High Performance Microelectronics IHP) and Dipl.-Ing. (FH) Kai Zoschke (Fraunhofer Institute for Reliability and Microintegration IZM).

Deutsche Kristallzüchtertagung 2021

Das IKZ hat schon oft Tagungen für die Kristallzüchter-Community veranstaltet. Für das Jahr 2021 hatten wir zugesagt, die jährlich an unterschiedlichen Orten stattfindende „Deutsche Kristallzüchtertagung“ der *Deutschen Gesellschaft für Kristallwachstum und Kristallzüchtung e.v.* (DGKK) zu organisieren und zu veranstalten. Hier treffen sich Kristallzüchter vorwiegend aus Deutschland, um die neuesten wissenschaftlichen Ergebnisse, Erfolge und Fragen zu diskutieren. Als Fachgesellschaft und Netzwerk ist die DGKK – und damit auch die Jahrestagung – für das IKZ von erheblicher wissenschaftsstrategischer Bedeutung. Schon im Vorfeld war klar, dass wir die Jahrestagung in Präsenz abhalten wollen. Deshalb wurde die Tagung aufgrund der Covid-19-Problematik von März auf Oktober 2021 verschoben.

Von 6. – 8. Oktober konnte die Jahrestagung DKT 2021 dann auch wirklich stattfinden. Unter Hygieneauflagen (Maskenpflicht, Abstandsregeln und Teilnehmerbegrenzung) trafen sich über 80 DGKK-Mitglieder und Interessierte. Mit dem direkt an das IKZ angrenzenden Max-Born-Saal wurde ein passender Tagungsraum gefunden. Am Tag zuvor hatte schon die „junge DGKK“ (jDGKK) in den gleichen Räumlichkeiten getagt. Die Tagungsorganisation und -leitung erfolgte durch Matthias Bickermann, R. Radhakrishnan Sumathi, Christiane Frank-Rotsch und Wolfram Miller vom IKZ. Trotz der Beschränkungen und Schwierigkeiten im Vorfeld konnten wir auch mehrere Firmen als Sponsoren und Aussteller für die Tagung gewinnen.

Am ersten Nachmittag wurden sieben Vorträge zur Züchtung von Massivkristallen gehalten. Die folgende Postersession wurde mit Kurzvorstellungen aller Poster durch die jeweiligen Präsentatoren eingeleitet, ein neues Element, dass auf sehr positive Resonanz gestoßen ist.

German Crystal Growers Conference 2021

The IKZ has often organized conferences for the crystal growing community. For 2021, we had agreed to organize and host the “German Crystal Growers Conference” of the German Society for Crystal Growth (DGKK), which takes place annually at different locations. Here crystal growers mainly from Germany meet to discuss the latest scientific results, achievements and issues. As a professional society and network, the DGKK – and thus also the annual meeting – is of considerable strategic scientific importance for the IKZ. From the beginning it was clear that we want to hold the annual meeting in presence. Due to the Covid 19 issue, the meeting was postponed from March to October 2021.

From October 6 – 8, the annual meeting DKT 2021 could then actually take place. More than 80 DGKK members and interested parties met under hygienic conditions (mandatory masks, distance rules and limitation of the number of participants). A suitable meeting room was found in the Max Born Hall, which is directly adjacent to the IKZ. The day before, the jDGKK had already met in the same rooms. The conference was organized and managed by Matthias Bickermann, R. Radhakrishnan Sumathi, Christiane Frank-Rotsch and Wolfram Miller from IKZ. Despite the initial limitations and difficulties, we were also able to attract several companies as sponsors and exhibitors for the conference.

On the first afternoon, seven lectures were given on the growth of bulk single crystals. The following poster session was introduced with short presentations of all posters by the respective presenters, a new element that met with a very positive response. On the same evening, the DGKK general assembly was held under the chairmanship of the (then vice) chairman of the DGKK, Andreas Erb. The meeting was significantly supported by Christiane Frank-Rotsch as acting DGKK secretary.

Am gleichen Abend fand bereits die Mitgliederversammlung unter Leitung des (damals stellvertretenden) Vorsitzenden der DGKK, Andreas Erb, statt. Die Sitzung wurde maßgeblich durch Christiane Frank-Rotsch als amtierende DGKK-Schriftführerin unterstützt. Matthias Bickermann wurde zum Wahlleiter bestellt und leitete die Neuwahlen des Vorstands. Zudem wurden neue DGKK-Ehrenmitglieder ernannt.

Thema des zweiten Tages war das epitaktische Wachstum von GaN mittels verschiedener Herstellungsmethoden. So berichtete z.B. Tim Wernicke als eingeladener Sprecher über die Herstellung von UV-LEDs, welche auf AlGaN basieren. Danach folgten Vorträge zur Kristallzüchtung für Detektoren im Bereich der Teilchenphysik.
Ein ganz wesentlicher Programmpunkt und eine Neuerung auf der DKT war eine Session mit dem Fokusthema „Technologiesouveränität" mit mehreren eingeladenen Sprechern aus der Industrie und aus Forschungsinstituten. Erörtert wurden hier vor allem die Wichtigkeit der Technologie und Methodik der Kristallzüchtung für den Standort Deutschland. Wirklich bemerkenswert war dabei das Aufzeigen von Materialtransfer und Wertschöpfung weltweit am Beispiel von GaAs für die Anwendung in Mobiltelefonen in einem Vortrag von Stefan Eichler (FCM). Durch die globale Vernetzung der Weltwirtschaft und international operierende Firmen laufen Deutschland und Europa Gefahr, sich von Risikogebieten, undemokratischen Staaten oder Billiglohnländern wirtschaftlich abhängig zu machen.
Diese „Fokus Session" stieß auf ein hohes Interesse und wurde als voller Erfolg gewertet. Dieses Format soll zukünftig beibehalten werden als exzellente Maßnahme, um Kontakt mit Industrie und Politik zu halten bzw. aufzubauen und insbesondere die Politik für strategische Herausforderungen in der Kristallzüchtung zu sensibilisieren.

Auf der traditionellen geselligen Abendveranstaltung wurden die von einer Jury bestimmten besten Posterpräsentationen ausgezeichnet und Kevin-Peter Gradwohl vom IKZ wurde für seine Arbeit zur Simulation der Versetzungsdynamik in Halbleitern der DGKK-Nachwuchspreis verliehen. Am Freitag, dem letzten Tag der DKT 2021, fanden noch dann noch weitere Vorträge zu verschiedenen Themen der Kristallzüchtung statt. Wir freuen uns sehr, dass die Veranstaltung in Präsenz, sowie die gesamte Organisation von vielen Teilnehmern so positiv aufgenommen wurde.

Matthias Bickermann was appointed election officer and presided over the new board elections. In addition, new DGKK honorary members were appointed.

On the second day, epitaxial growth of GaN using different fabrication methods was discussed. For example, Tim Wernicke, as an invited speaker, reported on the fabrication of UV LEDs based on AlGaN. This was followed by presentations on crystal growth for detectors in the field of particle physics.
A very important program item and an innovation at the DKT was a session with focus topic "Technology Sovereignty" comprised of several invited presentations from industry and research institutes. The main topic of discussion was the importance of the technology and methodology of crystal growth for Germany as a business location. Really remarkable was the presentation of material transfer and value creation worldwide using the example of GaAs for the application in cell phones in a lecture by Stefan Eichler (FCM). Due to the global networking of the world economy and internationally operating companies, Germany and Europe run the risk of becoming economically dependent on unstable world regions, undemocratic states or low-wage countries.
The "Focus Session" met with a high level of interest and was considered a complete success. This format is to be retained in the future as an excellent measure to maintain or establish contact with industry and politics and, in particular, to sensitize politics to strategic challenges in crystal growth.

At the traditional social evening event, the best poster presentations, as determined by a jury, were honored and the DGKK Young Scientist Award was presented to Kevin-Peter Gradwohl from IKZ for his work on the simulation of dislocation dynamics in semiconductors. On Friday, the last day of DKT 2021, there were more lectures on different topics of crystal growth. The successful organization and the event in presence was very positively emphasized by all attendees.

IKZ Stand, Ausstellung Naturkundemuseum im Rahmen der Berlin Science Week
IKZ booth at the Museum for Natural History during Berlin Science Week

Das IKZ auf der Berlin Science Week

Parallel zur Podiumsdiskussion Technologiesouveränität (s. Seite 14) präsentierte sich das IKZ mit einem Informationsstand im Naturkundemuseum im Rahmen der Berlin Science Week. Besucher des Gespräches zur Technologischen Souveränität konnten sich somit im Anschluss über das Institut informieren und im direkten Gespräch mit dem stellv. Direktor Prof. Dr. Matthias Bickermann die ein oder andere Frage besprechen. Aber auch allgemeine Besucher der Berlin Science Week nutzen die Gelegenheit, mehr über das IKZ zu erfahren.

The IKZ at the Berlin Science Week

Parallel to the panel discussion on technological sovereignty (see page 14), the IKZ presented itself with an information desk at the Museum of Natural History as part of the Berlin Science Week. Visitors of the discussion on technological sovereignty could inform themselves about the institute and discuss their questions with the deputy director Prof. Dr. Matthias Bickermann. But also general visitors of the Berlin Science Week took the opportunity to learn more about the IKZ.

VIDEO
www.ikz-berlin.de/oeffentlichkeitsarbeit/infos-fuer-medien-und-oeffentlichkeit-/-videos

David Uebel and Owen Ernst presenting a science clip of the IKZ
David Uebel und Owen Ernst zeigten einen Wissenschaftsfilm zum IKZ

Am Abend präsentierte Dr. Carsten Hucho vom PDI sowie der Unterhaltungskünstler Friedrich Lichtenstein die Wissenschaftsshow „Jetzt sprechen die Blumen“, wobei sich das IKZ mit Owen Ernst und David Uebel als einer der 3 Kandidaten mit einem Wissenschafts-Film präsentierte.

In the evening, Dr. Carsten Hucho from the PDI and entertainer Friedrich Lichtenstein presented the science show "Now the flowers are talking", with Owen Ernst and David Uebel presenting the IKZ as one of the 3 candidates with a science film.

Film zum Girls´Day – Vorstellung des IKZ
Girls'Day film – Presentation of the IKZ

Girls' Day 2021: Programm „Faszination Kristalle“ in neuem Format

Auch während der Corona-Pandemie sollten die jungen Frauen nicht auf die Möglichkeit verzichten müssen, unser Institut kennenzulernen und einiges über Kristallzüchtung zu erfahren. Demnach gab es 2021 zum ersten Mal ein digitales Format des Girls' Days am IKZ.

Die Mädchen im Alter zwischen 10 und 14 Jahren erhielten Einblicke in unsere Arbeit und lernten, wie Kristalle sie in ihrem täglichen Leben begleiten. Spannende Fragen, wie z.B. „Woraus besteht mein Handy?“ konnten geklärt und die vielen Einsatzmöglichkeiten von Kristallen diskutiert werden.

In Vorbereitung zum diesjährigen Girls´Day wurde extra hierfür ein Film produziert, sodass die Teilnehmerinnen u.a. digital durch das Institut geführt wurden und eine Czochralski-Züchtung aus nächster Nähe bestaunen konnten.

Girls' Day 2021: "Fascination Crystals" in a new format

Even during the Corona pandemic, young women should not have to miss the opportunity to get to know our institute and learn about crystal growth. Therefore, in 2021, the Girls' Day at the IKZ had a digital format for the first time.

The girls, aged between 10 and 14, were given insights into our work and learned how crystals accompany them in their daily lives. Exciting questions, such as "What is my cell phone made of?" could be answered and the many applications of crystals discussed.

In preparation for this year's Girls' Day, a film was produced especially for this purpose, so that the participants received, among other things, a digital tour of the institute and were able to see a Czochralski growth from close up.

Girls'Day
Mädchen-Zukunftstag

Nachwuchs
Young talents

Felix Mauerhoff erhält beim OPTICA Laser Congress 2021 gleich zwei Preise für den besten Studentenbeitrag

Für seine exzellente Präsentation zu den Ergebnissen seiner Forschung zur Festkörper-Laserkühlung von hochreinen Ytterbium-dotierten Calcium- und Strontiumfluorid-Kristallen erhielt Felix Mauerhoff neben dem begehrten „OPTICA Foundation Student Paper Award“ auch den mit 500 € dotierten „IPH Student Paper Award“ bei der „Advanced Solid State Lasers“ Konferenz im Rahmen des jährlichen OPTICA Laser Congress 2021.

Nachdem sich Felix Mauerhoff im Rahmen seiner Bachelorarbeit am IKZ mit der spektroskopischen Charakterisierung von Chrom-dotierten Fluorid-Kristallen sowie deren Einsatz als Verstärkermaterial in diodengepumpten Laserresonatoren beschäftigt hat, widmete er sich in seiner Masterarbeit der optischen Kühlung hochreiner Yb^{3+}-dotierter Fluoridkristalle durch Einstrahlung von Laserlicht.

F. Mauerhoff, S. Püschel, C. Kränkel, and H. Tanaka,
Laser Cooling of Yb^{3+}*-doped* CaF_2 *and* SrF_2 *Crystals*,
in *Laser Congress 2021 (ASSL,LAC)*,
(Optica Publishing Group, 2021), paper ATh1A.3,
https://doi.org/10.1364/ASSL.2021.ATh1A.3

Felix Mauerhoff wins two Student Paper Awards at OPTICA Laser Congress 2021

For his excellent presentation on the current results of his research on solid state laser cooling of high-purity ytterbium-doped calcium and strontium fluoride crystals, Felix Mauerhoff received the the ‘OPTICA Foundation Student Paper Award’ as well as the ‘Laser Congress IPH Student Paper Award’ with an endowment of 500 € for the best student paper at the ‘Advanced Solid State Lasers’ conference during the annual OPTICA Laser Congress 2021.

After Mr. Mauerhoff worked on his bachelor thesis at IKZ on the spectroscopic characterization of chromium-doped fluoride crystals and their use as amplifier material in diode-pumped lasers, his master thesis was dedicated to the optical cooling of Yb^{3+}-doped fluoride crystals by laser light irradiation.

F. Mauerhoff, S. Püschel, C. Kränkel, and H. Tanaka,
Laser Cooling of Yb^{3+}*-doped* CaF_2 *and* SrF_2 *Crystals*,
in *Laser Congress 2021 (ASSL,LAC)*,
(Optica Publishing Group, 2021), paper ATh1A.3,
https://doi.org/10.1364/ASSL.2021.ATh1A.3

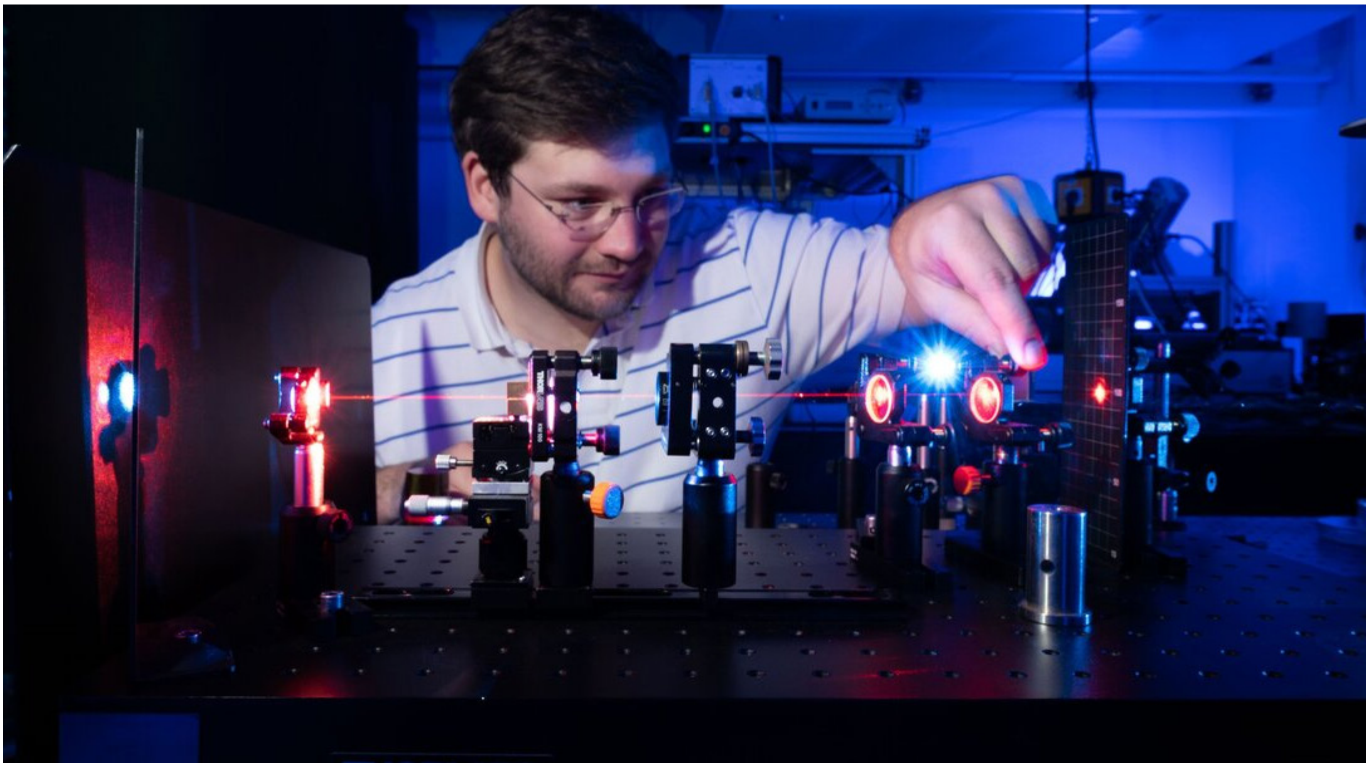


Foto: Prof. Dr. Georg Sommerer, Beuth Hochschule für Technik, Berlin

Zweifache Auszeichnung für Kevin-Peter Gradwohl

Für seine Forschung zur Defektcharakterisierung von hochreinen Germanium-Kristallen und dem Einfluss der Wachstumsrichtung auf deren Versetzungsstruktur wurde der IKZ-Doktorand Kevin-Peter Gradwohl in 2021 zweifach ausgezeichnet. So erhielt er sowohl den Young Scientist Award der 8th Asian Conference on Crystals Growth and Crystal Technology (CGCT), als auch den Nachwuchspreis der Deutschen Gesellschaft für Kristallzüchtung und Kristallwachstum (DGKK).

Seine Arbeiten an hochreinem Germanium sind eingebettet in das internationale Projekt LEGEND, in dem 50 Institutionen weltweit an der Aufklärung des neutrinolosen Doppelbeta-Zerfall von Germanium-76 forschen. Weitere Details zu der Forschung von Kevin-Peter Gradwohl finden sich auf Seite 42/43 bei den Berichten der Volumenkristalle.

K.-P. Gradwohl, U. Juda, and R.R. Sumathi; *The impact of the dislocation distribution and dislocation type on the charge carrier lifetime in Czochralski germanium single crystals*; Journal of Crystal Growth 573 (2021) 126285, https://doi.org/10.1016/j.jcrysgro.2021.126285

Double award for Kevin-Peter Gradwohl

For his research on the defect characterization of high-purity germanium crystals and the influence of the growth direction on their dislocation structure, IKZ doctoral student Kevin-Peter Gradwohl received two awards in 2021. He was awarded both the Young Scientist Award of the 8th Asian Conference on Crystals Growth and Crystal Technology (CGCT), and the Young Scientist Award of the German Society for Crystal Growth and Crystal Growth (DGKK).

His work on high-purity germanium is embedded in the international LEGEND collaboration, in which 50 institutions worldwide are conducting research to elucidate the neutrinoless double-beta decay of germanium-76. Further details on the research of Kevin-Peter Gradwohl can be found on page XX at the Volume Crystals section.

K.-P. Gradwohl, U. Juda, and R.R. Sumathi; *The impact of the dislocation distribution and dislocation type on the charge carrier lifetime in Czochralski germanium single crystals*; Journal of Crystal Growth 573 (2021) 126285, https://doi.org/10.1016/j.jcrysgro.2021.126285

Bericht der Promovierenden

Im zweiten Jahr mit Corona-Beschränkungen haben sich die Doktoranden weiter gut an die Situation angepasst: Effizient in den Laboren arbeiten und alle relevanten Daten sammeln, um diese dann im Homeoffice für Präsentationen und Paper aufzuarbeiten. Auf diese Weise konnten wir an vielen internationalen Konferenzen teilnehmen, ohne Berlin überhaupt zu verlassen. Ein Höhepunkt im Jahr 2021 war die DKT-Konferenz im IKZ, bei der einige von uns ihre Forschungsergebnisse zum ersten Mal einem „richtigen“ Publikum präsentieren konnten.

Auch bei Interaktion untereinander war das Motto Kontakte knüpfen aber Distanz halten. Das Doktorandenseminar musste größtenteils online abgehalten werden, aber in den warmen Monaten stand einem anschließenden Grillabend nichts im Wege. Ende November unternahmen wir eine Exkursion an die Universität Leipzig: Die Gruppe von Prof. von Wenckstern empfing uns in ihren Laboren und stieß auf großes Interesse an ihrer Forschung über kombinatorische Epitaxie. Ein anschließender Besuch des Leipziger Weihnachtsmarktes war leider nicht möglich – stattdessen ging es nach einem weihnachtlichem Stadtspaziergang zurück zum Bahnhof, wie man auf dem Bild sehen kann.

Im Jahr 2021 konnten wir neun neue Doktoranden an unserem Institut begrüßen, von denen zwei in Hamburg am DESY arbeiten. Sieben von uns haben ihre Dissertation erfolgreich verteidigt und damit die Gruppe der Doktoranden verlassen, um in Industrie oder Wissenschaft den nächsten Abschnitt zu beginnen. Ende 2021 sind Aykut Baki und Yujia Liu als Sprecher der Promovierenden zurückgetreten, um sich auf die Fertigstellung ihrer Arbeiten zu konzentrieren – vielen Dank für euer großes Engagement – und Stefan Püschel und Arved Enders-Seidlitz haben diese Aufgabe übernommen.

Wir freuen uns auf viele interessante Verteidigungen, motivierte neue Doktoranden und entspannte Grillabende im Jahr 2022!

Report of the doctoral students

The second year with Covid-19 regulations went by and we PhDs have adapted well to the situation: working hard in the labs to get all the relevant data which is then used to prepare presentations and write papers when being in the home office. In this way, we could contribute to many international conferences without even leaving Berlin. A highlight in 2021 was the DKT conference at IKZ held in presence, where some of us could present their research to a “real” audience for the first time.

Socializing yet distancing, was the key phrase when talking about interactions. The PhD seminar had to be held mostly online, but in the warm months nothing stood in the way of meeting outside for BBQ afterwards. At the end of November, we went on an excursion to Leipzig University: the group of Prof. von Wenckstern welcomed us in their labs and was met with much interest in their research about combinatorial epitaxy techniques. Unfortunately, the visit to the Christmas market afterwards was not possible – instead we had a nice walk through the city back to the train station, as you can see on the picture.

In 2021 we could welcome 9 new PhD students at our institute, two of them are working in Hamburg at the DESY. Seven of us successfully defended their thesis’ and, thus, left the PhD group for new jobs in industry or science. In the end of 2021, Aykut Baki and Yujia Liu stepped back from their work as PhD representatives to focus on finalizing their work – thanks for your great engagement – and Stefan Püschel and Arved Enders-Seidlitz took over.

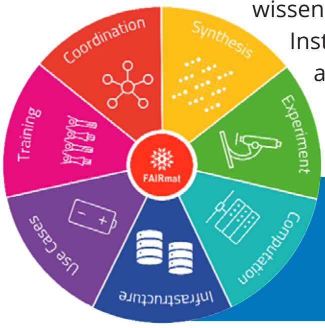
We are looking forward to many interesting defenses, motivated new PhD students and relaxed BBQ evenings in 2022!

Ausgewählte Projekte
Featured Projects

FAIRmat: Eine Schatzkiste voller Materialdaten

Der technologische Fortschritt in den Bereichen Energie, Umwelt, Gesundheit, Mobilität und Informationstechnik beruht auf der Entwicklung verbesserter oder neuartiger Materialien. Die enormen Mengen an Forschungsdaten, die täglich in diesem Bereich produziert werden, stellen eine „Goldmine des 21. Jahrhunderts“ dar, wenn sie leicht geteilt und mit Methoden der Datenanalyse und Methoden der Künstlichen Intelligenz bearbeitet werden könnten. Hierzu bedarf es einer effizienten und gut nutzbaren Forschungsdatenbank in der Daten FAIR, d.h. auffindbar (**F**indable), zugänglich (**A**ccessible), interoperabel (**I**nteroperable) und wiederverwendbar (**R**eusable) sind. Daten auffindbar and für künstliche Intelligenz bereit zu machen wird die Art und Weise, wie Wissenschaft betrieben wird, nachhaltig verändern.

Hier setzt FAIRmat (“FAIR Data Infrastructure for Condensed-Matter Physics and the Chemical Physics of Solids”) an. Das Projekt ist Teil der Nationalen Daten Infrastruktur (NFDI), eines bundesweites Netzwerks, welches von 2019 bis 2028 mit bis zu 90 Millionen Euro pro Jahr von Bund und Ländern gefördert wird. Am Konsortium unter Leitung der HU Berlin ist sind das Leibniz-Institut für Kristallzüchtung (IKZ), das Max Planck Institute for Chemical Energy Conversion (MPI CEC), das Fritz-Haber-Institut der Max-Planck-Gesellschaft (FHI), die Technische Universität München (TUM), das Karlsruher Institut für Technology (KIT) und der FAIR-DI e.V. als Mitantragsteller beteiligt. Das Projekt stützt sich auf die umfassenden Erfahrungen mit der weltweit größten Dateninfrastruktur der computergeschützten Materialwissenschaften, dem Novel Materials Discovery (NOMAD) Laboratory. FAIRmat hat sich zum Ziel gesetzt eine integrierten Dateninfrastruktur im Bereich Materialwissenschaften zu schaffen, die die Bereiche Synthese, experimentelle Materialwissenschaften und computergestützte Materialwissenschaften umfasst. Während der Laufzeit von fünf Jahren werden Forscherinnen und Forscher aus den Bereichen Datenwissenschaft, IT-Infrastruktur, Software-Engineering und den Materialwissenschaften aus 34 deutschen Institutionen in 60 Projekten als gleichberechtigte Partner im FAIRmat-Konsortium zusammenarbeiten.



Das IKZ verantwortet den Bereich der Materialsynthese und hat sich zum Ziel gesetzt die international erste umfassende Datenbank im Bereich der Materialsynthese zu realisieren.

FAIRmat: A treasure chest of material data

Technology progress in the fields of energy, environment, health, mobility and information technology is based on the development of improved or novel materials. The enormous amounts of research data produced daily in this field represent a “gold mine of the 21st century” if they could be easily shared and processed using data analysis and artificial intelligence methods. This requires an efficient and usable research database in which data is FAIR, i.e., **f**indable, **a**ccessible, **i**nteroperable, and **r**eusable. Making data findable and accessible to artificial intelligence will change the way science is done.

This is where FAIRmat (“FAIR Data Infrastructure for Condensed-Matter Physics and the Chemical Physics of Solids”) comes in. The project is part of the National Data Infrastructure (NFDI), a nationwide network funded by the federal and state governments with up to 90 million euros per year from 2019 to 2028. The consortium, led by HU Berlin, includes the Leibniz Institute for Crystal Growth (IKZ), the Max Planck Institute for Chemical Energy Conversion (MPI CEC), the Fritz Haber Institute of the Max Planck Society (FHI), the Technical University of Munich (TUM), the Karlsruhe Institute of Technology (KIT) and FAIR-DI e.V. as co-applicants. The project builds on extensive experience with the world’s largest data infrastructure in computational materials science, the Novel Materials Discovery (NOMAD) Laboratory. FAIRmat aims to create an integrated materials science data infrastructure spanning synthesis, experimental materials science, and computational materials science. During the five-year period, researchers from the fields of data science, IT infrastructure, software engineering and the materials sciences from 34 German institutions will collaborate in 60 projects as equal partners in the FAIRmat consortium. The IKZ is responsible for the area of materials synthesis and has set itself the goal of realizing the first internationally comprehensive database in the field of materials synthesis.

https://www.fair-di.eu/fairmat
https://www.dfg.de/foerderung/programme/nfdi/index.html
https://nomad-lab.eu
https://www.nature.com/articles/s41586-022-04501-x

IKZ Ausgründungen: Die Macht der Zeit –

Wie es zwei IKZ Wissenschaftlern gelang, die Zeitstruktur von Röntgenstrahlen zu kontrollieren

IKZ Spin-Off Companies: The Power of Time –

How two IKZ scientists succeeded in controlling the time structure of X-rays

Foto: Leo S. Koch von Hamburg Innovation

ein Interview mit / an interview with
Dr. Peter Gaal & Daniel Schmidt,
Gründer von TXproducts /
founders of TXproducts

Das Interview führte / The interview was conducted by Stefanie Grüber

Wie schön wäre es, Röntgenstrahlen zeitlich so zu kontrollieren, dass diese genau dann in der gewünschten Dauer auftreten, wenn man es möchte. Dies würde einen enormen Fortschritt für Forschende bedeuten, die an hochintensiven Röntgenquellen arbeiten, den sogenannten Synchrotrons. Mithilfe dieser Lichtquellen können die Wissenschaftlerinnen und Wissenschaftler an den Experimentierstationen unterschiedlichste Phänomene aus verschiedenen wissenschaftlichen Disziplinen untersuchen. An einem Synchrotron werden ca. 20-40 Experimente gleichzeitig betrieben, von denen alle dieselbe Strahlung nutzen. Leider ist das zeitliche Muster dieser Strahlung aber nicht für alle Nutzerinnen und Nutzer individuell anpassbar. Lange Wartezeiten auf einen bestimmten Betriebsmodus oder hoher instrumenteller Aufwand sind die Folge. Im Gegensatz zur Photonenenergie oder der Strahlgröße konnte die Zeitstruktur bisher noch nicht mit Optiken gezielt eingestellt werden. Genau dieser Herausforderung haben sich Dr. Peter Gaal, Leiter der Gruppe Röntgenoptik am IKZ sowie Leiter des Joint Lab IKZ-DESY in Hamburg, und Daniel Schmidt, studierter Nanowissenschaftler und Mitarbeiter in der Gruppe Röntgenoptik, angenommen. Was zunächst nur eine Idee war, wurde von den beiden in einem Zwei-Mann-Startup namens *TXproducts* erfolgreich zur Marktreife geführt.

Imagine how wonderful it would be to control the timing of X-rays so that they occur for exactly the desired duration whenever you want them to. This would mean an enormous advance for researchers working on high-intensity X-ray sources, the so-called synchrotrons. Such light sources enable researchers at the experimental stations to study a wide variety of phenomena from different scientific disciplines. Approximately 20-40 experiments are carried out at one synchrotron at the same time, and they all use the same radiation. Unfortunately, the time pattern of this radiation cannot be adapted individually for all users. This results in long waiting times for a certain operating mode or high instrumental effort. Unlike photon energy or beam size, the time structure could not be specifically adjusted with optics until now. This was exactly the challenge that Dr. Peter Gaal, head of the X-ray optics group at the IKZ and head of the Joint Lab IKZ-DESY in Hamburg, and Daniel Schmidt, a specialist in nanoscience research and member of the X-ray optics group, took on. Initially just an idea, this was successfully brought to market by the two scientists in a two-man startup called *TXproducts*.

Aber was genau macht euer Gerät?

Peter Gaal: *Unser Hauptprodukt ist ein Röntgen-Chopper, also ein Gerät, das auf Kommando Röntgenstrahlung durchlässt oder eben nicht. Einen Röntgenstrahl zu blocken ist erst einmal keine leichte Aufgabe, denn Röntgenstrahlung ist vor allem für ihr hohes Durchdringungsvermögen bekannt. An der schnellen Manipulation der Zeitstruktur von Synchrotronstrahlung wird seit rund 30 Jahren geforscht, also im Grunde, seit es Synchrotrons für die Forschung gibt. Und mit schnell meinen wir tatsächlich innerhalb von wenigen Nanosekunden. Und unser Gerät macht genau das. Mithilfe eines Steuersignals kann man sagen: ´Mach den Strahl 100 Nanosekunden auf und mach ihn dann wieder zu´. Diesen Vorgang kann man beliebig oft wiederholen. Genau, wie man es eben* für *ein Experiment benötigt. Man kann den Strahl aber nicht nur* für *100 Nanosekunden auf und wieder zu machen, sondern auch* für *Mikrosekunden, Millisekunden, Minuten oder Stunden. Mithilfe dieses Gerätes kann sozusagen das komplette Zeitverhalten* der Röntgenstrahlen *kontrolliert werden.*

Und wo genau kommt euer Gerät zum Einsatz?

Peter Gaal: *In erster Linie ist es ein Gerät* für das *Synchrotron. Jedes Experiment an einer Beamline ist einzigartig und genauso groß sind auch die Anwendungsfelder unseres Choppers. Ein gutes Beispiel* für unseren Chopper ist *die Protein-Kristallographie, die fast die Hälfte der Kristallographie-Experimente an Synchrotrons ausmacht. Oft besteht das Problem, dass der Protein-Kristall durch den Strahl kaputt geht. Um die wertvollen Proben zu schonen, möchte man sie nur dann dem Strahl aussetzen, wenn auch tatsächlich gemessen wird, und nicht wenn z.B. der Detektor ausgelesen wird. Ein aktuelles Beispiel ist hier das Coronavirus, das man intensiv am Synchrotron untersucht hat. Für diese Fälle* könnte man unseren Schalter einsetzen. *Es gibt aber auch eine Vielzahl anderer Anwendungen, z.B. dynamische Prozesse, die man untersuchen möchte. Oftmals ist das normale Mess-Equipment nicht schnell genug, um die Dynamik aufzulösen. Eine mögliche Lösung besteht dann darin, den Röntgenpuls kurz zu machen. Die Belichtungszeit einer Röntgenkamera kann man z.B. nicht beliebig kurz einstellen, weil das durch die Schaltelektronik begrenzt ist. Um einen besonders schnellen Prozess beobachten zu können, muss stattdessen der Röntgenpuls kurz sein. Und hier kommt wieder unser Chopper ins Spiel.*

Daniel Schmidt: *Aber wo die Reise am Ende wirklich hingeht, ist noch nicht final geklärt. Wir hatten z.B. auch Anfragen aus der Medizin* für *Prototypen-Projekte. Soll heißen, wir wollen das Produkt nicht auf Anwendungen an Synchrotrons begrenzen. Wenn sich andere Bereiche auftun, dann werden wir diese natürlich auch bedienen.*

Foto: Leo S. Koch von Hamburg Innovation

But what exactly does your device do?

Peter Gaal: *Our main product is an X-ray chopper, in other words, a device that allows X-rays to pass through or not on cue. It is not an easy task to block an X-ray beam because X-rays are known for their high penetration power. Scientists have been working on the fast manipulation of the time structure of synchrotron radiation for about 30 years, so basically since synchrotrons have been available for research. And when we say fast, we actually mean within a few nanoseconds. Our device can do exactly that. You can use a control signal to say, 'Open the beam for 100 nanoseconds and then close it again'. This process can be repeated as often as you like. Just the way you need it for an experiment. Moreover, the beam can be opened and closed not only for 100 nanoseconds but also for microseconds, milliseconds, minutes or hours. So, it is possible to control the complete time behavior of X-rays with this device.*

And where exactly is your device used?

Peter Gaal: *In the first place, the device is intended for the synchrotron. Each experiment at a beamline is unique and the application fields of our chopper are just as diverse. A good example of our chopper is protein crystallography, which accounts for almost half of the crystallography experiments at synchrotrons. More often than not, the problem is that the protein crystal is broken by the beam. In order to avoid damaging the valuable samples, the researchers only want to expose them to the beam when they are actually measuring, and not when the detector is being read out, for example. A current case in point is the corona virus, which has been intensively studied at the synchrotron. For such cases, our switch could be used. There is, however, a multitude of other applications, such as dynamic processes that you might want to investigate. Standard measurement equipment is often not fast enough to resolve the dynamics. One possible solution then is to keep the X-ray pulse short. The exposure time of an X-ray camera, for example,*

Also auch medizinische Produkte sind nicht ausgeschlossen?

Daniel Schmidt: *Nein, das nicht. Aber aktuell ist es eher noch medizinische Forschung. Z.B. gibt es neue Verfahren für die Bestrahlung von Krebs (Radiation Therapy). Hier ist es sehr wichtig, dass nur das bestrahlt wird, was auch bestrahlt werden soll, und zwar nur dann, wenn der Arzt es möchte.*

Damit sind wir bei der klassischen Frage: Wo seht ihr euch in 5-10 Jahren? Welche neuen Felder könnten in Frage kommen?

Peter Gaal: *Wir möchten in erster Linie unsere Technologie der Aktiven Röntgenoptiken an Synchrotrons etablieren. Da ist zum einen der bereits erwähnte Chopper, es gibt aber noch weitere Optiken, die wir bauen oder deren Entwicklung wir derzeit vorantreiben. Mittelfristig möchten wir unsere Technologie aber auch in anderen Gebieten zum Einsatz bringen. Die gleichen physikalischen Prinzipien, die wir in unseren Aktiven Optiken anwenden, könnte man auch nutzen, um quantentechnologische Prozesse zu steuern oder um Nanoteilchen zu manipulieren. Hier befinden wir uns jedoch bislang im Entwicklungsstadium.*

Aber natürlich möchten wir auch personell wachsen. Derzeit sind wir mit unseren Synchrotronanwendungen absolut ausgelastet. Wenn sich unsere Technologie etabliert hat, möchten wir diesen Bereich in Zukunft gerne an neue Kolleginnen oder Kollegen abgeben und uns wieder mehr der Forschung an neuen Applikationen widmen. Wir sind bereits jetzt auf der Suche nach Studierenden, die vielleicht ihre Bachelor- oder Masterarbeit bei uns absolvieren möchten, gerne auch im Hinblick auf eine spätere Promotion. Aber auch Werkstudenten sind herzlich willkommen. Idealerweise bleiben die Studierenden dann bei uns und treiben das Unternehmen weiter voran.

Ihr habt also Großes vor. Doch wie ist die Idee überhaupt entstanden, sich auszugründen?

Peter Gaal: *Ich fand es schon immer spannend. Seitdem ich mit dem schnellen Röntgenschalter, also dem Pico-Switch, angefangen habe, wollte ich ein Unternehmen daraus machen. Das war vor ungefähr 10 Jahren. Jedoch ist es mehr Arbeit, als man denkt. Und ich habe leider auch keinen betriebswirtschaftlichen Hintergrund. Das kann man zwar alles lernen, aber wie so oft, fehlt einem die Zeit dafür. Aber dann kam Daniel als Student mit in meine Gruppe und hatte den gleichen Drive. Er wollte dasselbe wie ich und zu zweit ist vieles einfacher. Hinzu kam, dass uns Thomas Schröder (wissenschaftlicher Direktor des IKZ, A.d.R.) unterstützt hat und von der Idee überzeugt war.*

cannot be set as short as desired because this is limited by its electronic system. For observing a particularly fast process, the X-ray pulse has to be rather short instead. And this is where our chopper comes into play again.

Daniel Schmidt: *But where the journey will really take us is still completely open. We have had inquiries – for example – from the medical sector for prototype projects. What I mean is that we don't want to limit the product to applications on synchrotrons. If there are other areas that open up, we will certainly be willing to look into them as well.*

So, you don't exclude medical products either?

Daniel Schmidt: *No, we don't. However, for the time being it is still medical research. There are, for example, new procedures for the irradiation of cancer (radiation therapy). There it is very important to irradiate only what should be irradiated, and that only if the doctor wants it.*

Which brings us to the classic question: Where do you see yourselves in 5-10 years? And what new fields might be interesting for you?

Peter Gaal: *Our primary goal is to establish our technology of active X-ray optics at synchrotrons. There is the aforementioned chopper but there are also other optical components that we are building or whose development we are currently advancing. In the medium term, we would like to apply our technology in other fields as well. The same physical principles applied in our active optics could also be used to control quantum technological processes or to manipulate nanoparticles. However, we are still in the development stage here.*

We naturally also want to grow in terms of personnel. At the moment, our capacities are fully utilized with our synchrotron applications. Once we have established our technology, we would like to hand over this area to new colleagues in the future and dedicate ourselves more to research on new applications. We are already looking for students who may be interested in doing their bachelor's or master's thesis with us, also with a view to a doctorate later on. Working students are welcome, too. In the best of cases, the students will stay with us and drive the company forward.

I see you have big plans for the future. But how did the idea to spin off come about in the first place?

Peter Gaal: *It was something I always found exciting. Ever since I started with the fast X-ray switch, the PicoSwitch, I wanted to establish a company around it.*

Über das am DESY angesiedelte Joint Lab hatten wir eine direkte Verbindung zu einem wichtigen Partner. Besonders geholfen hat uns auch die Teilnahme am sogenannten Business Sprint. Das sind konzertierte Block-Seminare, in denen man in festgelegten Schritten durch den Gründungsprozess geführt wird. Die Gründung selbst mit allem Drum und Dran, dauerte dann doch relativ lange. Aber als wir gemerkt haben, dass aus der Idee etwas werden kann, wollten wir diese unbedingt umsetzen. Natürlich gab es auch Unsicherheiten: Wie sieht unser Markt aus? Wie lege ich den Preis für mein Produkt fest? Wie fange ich an, Kunden anzusprechen? Wie überzeuge ich die Kunden? Dieser Business Sprint hat uns bei diesen Fragen enorm weitergeholfen. Und dann hat man irgendwann gesehen, „Ja, das passt, das funktioniert alles". Und dann haben wir es einfach gemacht.

Gab es außerhalb des Business Sprints Unterstützung, die ihr erhalten habt?

Peter Gaal: *Der Workshop hat uns schon sehr weitergeholfen. Was ich aber auch erwähnenswert finde, sind die sogenannten „Wirtschaftssenioren" in Hamburg. Das sind erfahrene Manager, die keine Lust auf Ruhestand haben. Stattdessen beraten sie Startups, was für uns durchaus sehr hilfreich war. Wir konnten Fragen zu Finanzierungen und zum Businessplan diskutieren bis hin zu konkreten Fragen, z.B. zu Geschäftsbeziehungen in China. Aber man muss auch klar sagen, dass es uns nicht geben würde, wenn das IKZ nicht von der Idee überzeugt gewesen wäre und die Ausgründung nicht unterstützt hätte.*

Kann man denn sagen, wie lange der Prozess zwischen der Entscheidung, es aktiv anzupacken und sich letztendlich auszugründen, gedauert hat?

Daniel Schmidt: *Leider kam bei uns, wie bei so vielen, die Corona-Pandemie dazwischen. Insgesamt hat es gut ein Jahr gedauert. Am Ende vom Business Sprint haben wir angefangen, aktive Schritte für die Gründung zu unternehmen. Jedoch nahmen Dinge wie Notar, Beantragungen, Eintragungen etc. nochmals gut ein halbes Jahr in Anspruch. Hier braucht man eine größere Portion Geduld. Im Oktober 2021 waren wir dann als Unternehmen endlich in der Lage, unsere Geschäftstätigkeit aufzunehmen.*

That was about 10 years ago. However, it is more work than you can imagine. And unfortunately, I haven't got a business management background, either. Of course, you can learn all that but as is often the case, you don't have the time. But then Daniel joined my group as a student and had the same motivation. He wanted the same thing, and many things are easier if you do it together. Another important factor was that Thomas Schröder (Scientific Director of the IKZ, editor's note) supported us and was convinced of the idea.

We had a direct connection to an important partner via the Joint Lab located at DESY. Our participation in the so-called Business Sprint was also particularly helpful. This is a concerted series of block seminars in which you are guided through the startup process in defined steps. The process of setting up the company itself, with all the trimmings, took a relatively long time, though. But when we realized that the idea could become viable, we really wanted to put it into practice. There were, of course, uncertainties as well: What does our market look like? How do I determine the price for my product? How do I start approaching customers? How do I convince customers? For us, Business Sprint was a great help in answering these questions. There was a point when we saw, "Yes, this feels right – everything is going to work out". And then we just did it.

Did you receive any support apart from Business Sprint?

Peter Gaal: *The workshop really helped us a lot. But the so-called "Wirtschaftssenioren" in Hamburg also deserve a mention. These are experienced managers who have no desire to retire but advise startups instead. This definitely proved to be very helpful for us. We were able to discuss issues ranging from financing and the business plan to specific questions, such as business relations in China. However, it must also be clearly pointed out that we would not have been here if the IKZ had not been convinced of the idea and had not supported the spin-off.*

So is there any way of telling how long the process took from the decision to actively pursue the project to the eventual spin-off?

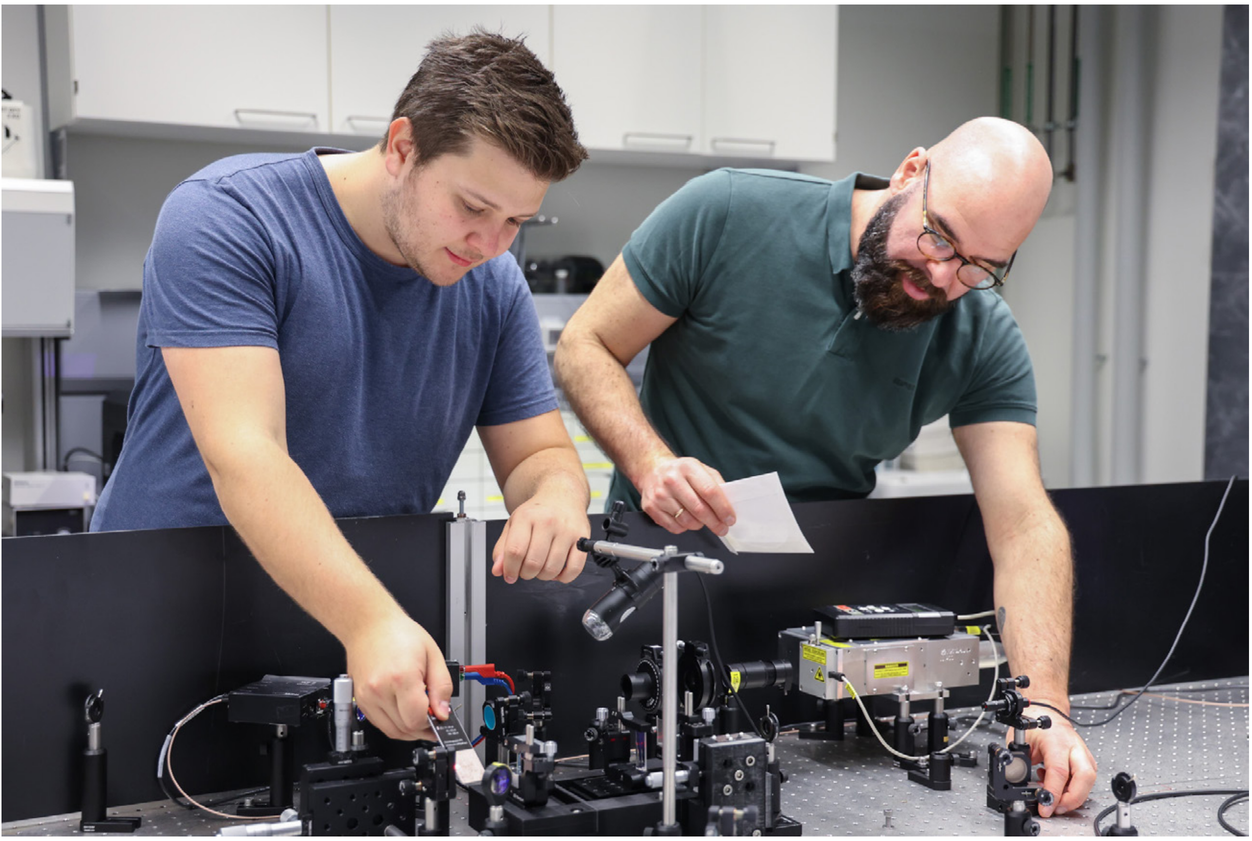
Daniel Schmidt: *Unfortunately, the Covid-19 pandemic got in the way, as it did for so many of us. All in all, it took a good year. At the end of the Business Sprint, we started to take active steps for founding the company. However, notary, applications, registrations, etc. took another six months. This really requires a great deal of patience. In October 2021, we were finally ready to start our business as a company.*

Was würdet ihr anderen mit auf den Weg geben wollen, die die Absicht haben, sich auszugründen?

Daniel Schmidt: *Grundsätzlich möchten wir Menschen dazu ermutigen. Ich glaube, es gibt viele Ideen, die in den Instituten rumliegen und nur darauf warten, weitergetrieben zu werden. Natürlich ist es auch immer ein wenig eine Frage des Glücks, die richtigen Leute zur richtigen Zeit zu finden. Aber es ist machbar und es lohnt sich. Auch denke ich, dass es von extremer Wichtigkeit ist, mit Menschen zu reden, die Erfahrungen haben oder Ähnliches vorhaben. Wenn also neue Ideen aus dem IKZ kommen, die nur darauf warten, umgesetzt zu werden, sprecht uns gerne an. Wir haben den Prozess gerade hinter uns und freuen uns, andere dabei zu unterstützen.*

What advice would you like to give to other people who are thinking of starting their own spin-off business?

Daniel Schmidt: *We would basically like to encourage people to do this. I believe there are many ideas just lying around in institutes, simply waiting to be developed. It is, of course, also always a bit of a question of luck to find the right people at the right time. But it is feasible and it is worth it. I also think it is of extreme importance to talk to people who have experience or similar plans. So, if there are new ideas coming from the IKZ and just waiting to be implemented, feel free to reach out to us. We have gone through the whole process right now and are happy to help others along the way.*



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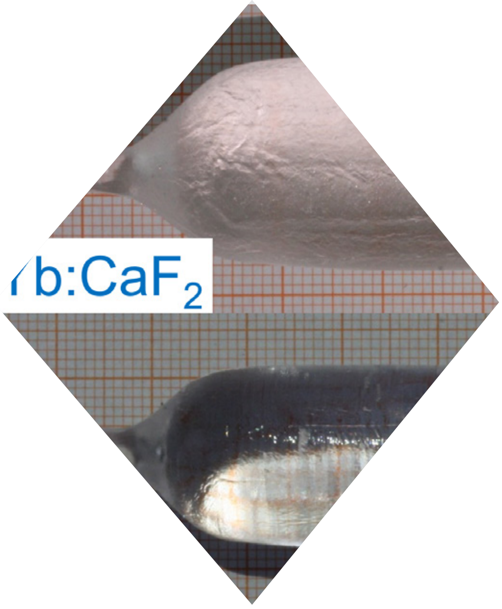

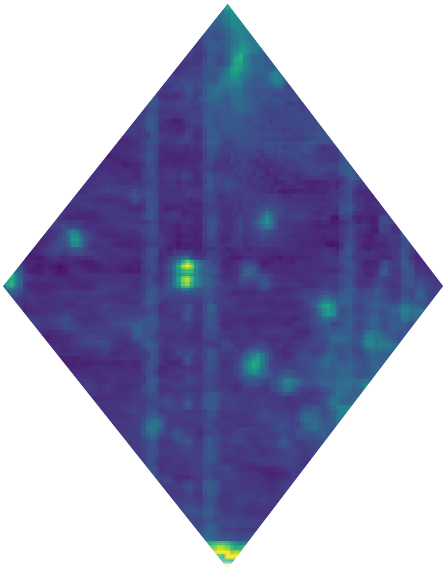

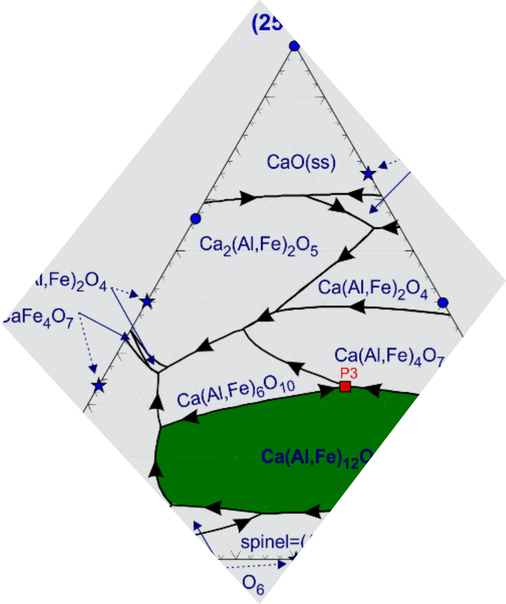

Volume Crystals

Efficient laser cooling in ytterbium-doped CaF_2 and SrF_2

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Laser cooling of solids is a unique approach to freeze lattice vibrations, *i.e.*, phonons, in solid phase materials. Some optically active materials, including rare-earth-doped crystals and glasses, exhibit absorption at energies below their mean fluorescence photon energy. Thus, when the low-energy edge of their absorption band is optically excited *e.g.* by lasers, the emitted photons have on average an energy higher than the excitation photons. This excess energy is provided by lattice phonons. In other words, this so-called anti-Stokes fluorescence "*consumes*" the energy of phonons, and consequently, the material cools by simple laser irradiation.

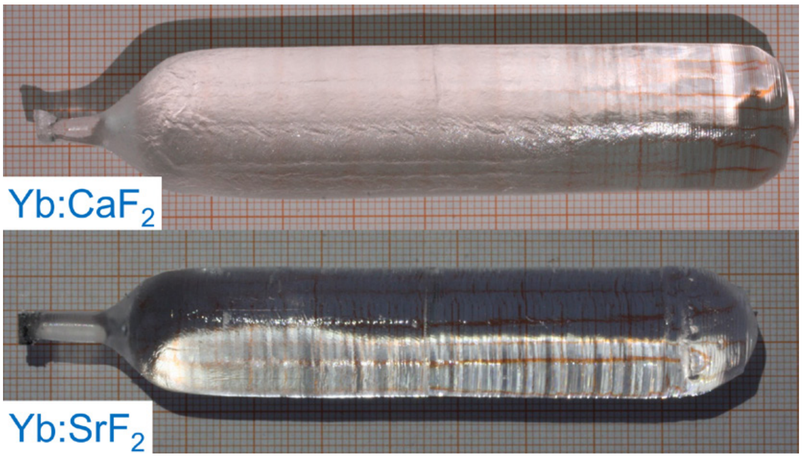
The demand of cooling is ubiquitous in experiments and devices in various fields. Current cooling techniques rely on the thermo-electric effect, cryogenic liquids, or thermodynamic refrigeration cycles. Laser cooling of solids enables to realize *all-solid-state optical cryocoolers* reaching temperatures below the limit of thermo-electric coolers at 175 K. Optical cryocoolers are intrinsically free of vibrations and can be very compact. Due to these unique advantages, they are of particular interest for high precision metrology and space-born devices.

Fluoride crystals doped with trivalent ytterbium (Yb^{3+}) are state-of-the-art laser cooling media, because their relatively low phonon energies avoid parasitic heating by multi-phonon relaxation processes. The most mature laser cooling medium, Yb^{3+}-doped $LiYF_4$ (Yb:YLF), achieved temperatures below 100 K [1]. To reach 77 K, which is an important milestone to replace liquid-nitrogen-based coolers [2], a further reduction of impurities was identified as a fundamental challenge. However, the variety of materials investigated for the purpose of laser cooling is very limited, to date. Thus, other fluoride crystals may have the potential to outperform Yb:YLF as laser cooling media.

In 2020, the junior research group '*Fluoride Single Crystals for Photonics*' headed by Dr. Hiroki Tanaka started its research work in this field, benefiting from the close collaboration of the section Oxides & Fluorides with the Center for Laser Materials at the IKZ. This intra-institutional and interdisciplinary collaboration provides an ideal environment for research on laser cooling of solids: crystal growth, spectroscopic characterization, and laser cooling experiments are all performed in-house.

Fluorite-type crystals are nowadays widely used for optics. For instance, CaF_2 is an important optical material due to its broad transparency range from the UV to mid-infrared. Furthermore, CaF_2 doped with rare-earth ions is a well-known laser gain medium for ultrafast laser oscillators and amplifiers. We grew CaF_2 and SrF_2 single crystals doped with 5% of Yb^{3+} (hereafter, Yb:CaF_2 and Yb:SrF_2) by the Czochralski method (cf. Fig. 1). The dimensions of both boules were 20 mm in diameter and ≈100 mm in length. The formation of Yb^{2+} was prevented by CF_4 in the growth atmosphere as confirmed by the absence of the characteristic UV absorption originating from the $4f^{14} \rightarrow 4f^{13}5d^1$ transition in Yb^{2+}.

Fig. 1 Czochralski-grown Yb^{3+}-doped CaF_2 (top) and SrF_2 (bottom) crystals.



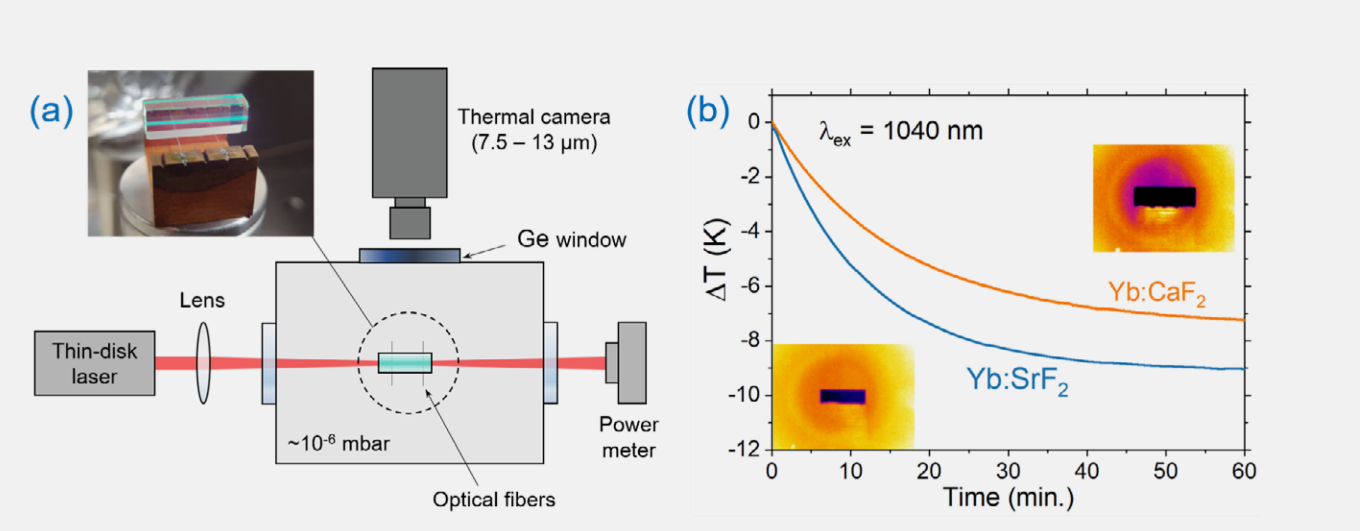


Fig. 2

(a) Schematic of the setup for laser cooling characterization. The photograph shows an irradiated Yb:CaF_2 crystal placed on two optical fibers.

(b) Recorded temperature change of the Yb:CaF_2 and Yb:SrF_2 under 1040-nm excitation with corresponding thermal camera images. The dark rectangles in the images are the crystals cooler than the surroundings

Figure 2 illustrates the experimental setup to characterize the laser cooling performance. Samples prepared from each boule were placed in a vacuum chamber to avoid convective heating from the surrounding. As shown in the photograph in Fig. 2(a), the samples were placed on two optical fibers with minimal contact areas to also minimize conductive heat exchange. The excitation source, an Yb:$Lu_3Al_5O_{12}$ thin-disk laser tunable from 990 to 1080 nm, was focused loosely into the laser cooling samples. The temperature of the samples was monitored by a thermal camera through a germanium window transparent for the camera's detection range 7.5–13 µm. Figure 2(b) shows the temperature change over time in Yb:CaF_2 and Yb:SrF_2 under 1.8-W single-pass excitation at 1040 nm.

Cooling was observed for a wide range of excitation wavelengths from 1018 to 1083 nm for Yb:CaF_2 and from 1014 to 1075 nm for Yb:SrF_2. The maximum cooling efficiency at room temperature was determined to be ≈3% for both crystals. We evaluated the external quantum efficiency to be as high as ≈98% and the background (or parasitic) absorption coefficient to be as low as ≈10^{-4} cm^{-1}. The obtained cooling efficiencies as well as the amount of background absorption were both comparable with the results reported for state-of-the-art Yb:YLF crystals.

The temperature-dependent spectroscopic data enabled to estimate the minimum achievable temperatures (MATs) to be 142 K for Yb:CaF_2 and 152 K for Yb:SrF_2 The optimum excitation wavelength to reach the MAT is ≈1030 nm for both crystals. This means that optical cryocoolers based on Yb^{3+}-doped fluorite-type crystals could strongly benefit from the availability of high-power Yb^{3+}-laser sources emitting at 1030 nm. More details on the characterization are found in our recent publication [3].

In conclusion, we unveiled the promising laser cooling ability of Yb^{3+}-doped fluorite-type crystals. The obtained cooling performances are comparable with state-of-the-art results achieved with Yb:YLF. Further improvement of the cooling efficiency as well as reduction of the MAT are feasible by using crystals of higher Yb^{3+} concentrations. Corresponding growth experiments are in progress and high-power laser cooling experiments are planned for the near future.

Acknowledgement

We thank the crystal preparation workshop at the IKZ for cutting and polishing of the Yb:CaF_2 and Yb:SrF_2 crystals used in this work.

References

[1] S. D. Melgaard, A. R. Albrecht, M. P. Hehlen, and M. Sheik-Bahae: Sci. Rep. 6, 2 (2016).

[2] M. P. Hehlen, J. Meng, A. R. Albrecht, E. R. Lee, A. Gragossian, S. P. Love, C. E. Hamilton, R. I. Epstein, and M. Sheik-Bahae: Light Sci. Appl. 7, 15 (2018).

[3] S. Püschel, F. Mauerhoff, C. Kränkel, and H. Tanaka: Opt. Lett. 47, 333 (2022).

Hexagallate substrates for oxide spintronic applications

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In the past, passive and active radio-frequency and microwave devices were based on magnetic materials such as microwave ferrites using magnetic spin waves as active medium. The next generation of microwave and millimeter-wave devices, for example for microwave signal processing, has been discussed more recently in the literature. However, it was the discovery that ferrites are able of transmitting electrical signals by converting them into spin waves [1] that opened the way for spin waves as data carriers in novel computing devices. These are the counterparts to electrons as data carriers in conventional electronics [2]. In the future, modern information and communication technologies will require frequency bandwidths from ~600 MHz up to several terahertz for ultra-fast, low-cost and environmentally friendly data processing. For these challenges, magnetic materials such as single-crystalline barium hexaferrite films are attractive. To achieve epitaxial films with excellent structural and magnetic perfection, a suitable substrate material with small lattice mismatch is required. In the case of barium hexaferrite ($BaFe_{12}O_{19}$) liquid phase epitaxy (LPE), alkali earth hexagallates are the materials of choice, because it has already been demonstrated that epitaxial films with high crystal quality can be grown on these substrates [3]. If high-quality films could be also grown by molecular beam epitaxy (MBE), it would bring an opportunity to engineer the properties of hexaferrites using strain engineering and other thin film approaches that have proven to be quite useful for enhancing the properties of other oxides or even accessing the properties of metastable polymorphs.

The substrates and epitaxial films of interest crystallize in the magnetoplumbite structure (space group: $P6_3/mmc$) with the general formula $AB_{12}O_{19}$. Here A (coordination number 12) is a large cation, like K^+, Pb^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}. B is a highly charged cation of intermediate size. Because as much as 5 non-equivalent B sites with coordination numbers from 4 to 6 exist in the hexagonal structure, a big variety of metals can occupy this position. Mateika and Laurien gave the first report on the bulk growth of a magnetoplumbite single crystal [4]. This was the “hexagallate” $SrGa_{12}O_{19}$ which melts peritectically and must be grown from melt solutions with SrO excess. Unfortunately, the growth window from which this phase crystallizes is very narrow; but they could increase the yield significantly by an equimolar partial substitution of Ga^{3+} with Mg^{2+} and Zr^{4+}. Recently, we could show that the Mg^{2+}/Zr^{4+} co-doping is so effective, because it widens the crystallization window for the hexagallate [5]. Meanwhile, high-quality bulk crystals of $(Mg,Zr):SrGa_{12}O_{19}$ (Fig. 1a) with diameters close to one inch were grown at IKZ in the frame of the activities of the Cornell-IKZ joint lab [10] and first batches of substrates (Fig. 1b) with various sizes were prepared by the company CrysTec GmbH. A novel X-ray diffraction rocking curve imaging procedure specifically developed for SGMZ reveals that the rocking curve widths are typically below 23 arcsec [6]. Therefore, the SGMZ crystals are largely homogeneous and hence suitable for the preparation of high-quality substrates.

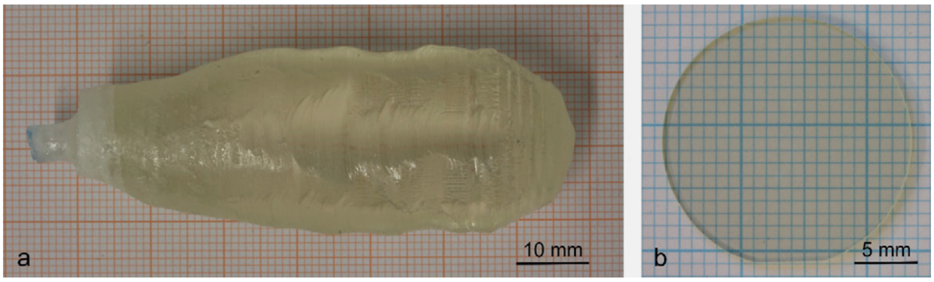

Fig. 1
(a) Most recent SGMZ single crystal grown by the top-seeded solution growth technique (TSSG) and (b) prepared chemo-mechanically polished (CMP) substrate with a diameter of 20 mm.

In order to explain the pioneering approach of Mateika and Laurien more vividly and to elucidate the widening of the crystallization window, we introduce the concentration triangle that is shown in Figure 2. The $CaO–Al_2O_3–Fe_2O_3$ system shown there has the benefit that it is much better investigated than the systems with Ga^{3+}, but behaves similar. Hence, it can be considered as a model system for future magnetoplumbite crystal growth experiments. Also, with the smaller cations Ca^{2+} and Al^{3+}, the magnetoplumbite $CaAl_{12}O_{19}$ is formed, and this composition is shown as a green asterisk on the $CaO–Al_2O_3$ rim. Al^{3+} can be partially substituted by Fe^{3+}, and the primary crystallization field of these mixed crystals is shown in green color, too. In analogy to the $SrO–Ga_2O_3$ system, the crystallization window for $CaAl_{12}O_{19}$ is narrow on the $CaO–Al_2O_3$ rim (from P1 at 23.4% to E1 at 29.7% CaO, with a temperature difference $DT = 79$ K). $Ca(Al,Fe)_{12}O_{19}$ mixed crystals, instead, possess a significantly increased primary crystallization field, which is limited, e.g., by the ternary invariant points P2 and P3. The distance between these points is >24% with respect to the CaO concentration, and >160 K with respect to the liquidus temperature.

Our recent publication [5] showed that co-doping with Mg and Zr widened the crystallization window for $SrGa_{12}O_{19}$ by two effects: (1) The lower limit, which is in the $CaO-Al_2O_3-Fe_2O_3$ system E1, was lowered by 20 K. This effect was expected, because eutectics of multi-component systems are usually lower, compared to binary systems. (2) The upper limit, here the peritectic decomposition of $CaAl_{12}O_{19}$, rises more than 60 K, because doping stabilized the magnetoplumbite phase. In total, the crystallization window could be widened from approx. $\Delta T = 35$ K to 120 K.

In Figure 2, the upper stability limit of the magnetoplumbite cannot be increased by Fe^{3+} doping, because the point of lowest liquidus temperature of the whole ternary system (1142°C), namely the ternary eutectic $Ca(Al,Fe)_2O_4/Ca(Al,Fe)_6O_{10}/Ca_2(Al/Fe)_2O_5$, is situated in the vicinity of its crystallization field. Consequently, Fe^{3+} doping alone simply reduces the liquidus temperature. Especially in the magnetoplumbite structure with as much as 5 non-equivalent B sites, co-doping with multiple ions, like introduced by Mateika & Laurien [4], increases the entropy much. This stabilizes the phase significantly.

Work on magnetoplumbite crystal growth and characterization will be continued. It is intended to introduce other, and possibly more metal ions into the structure – with the aim to adjust the lattice parameters for the desired substrates.

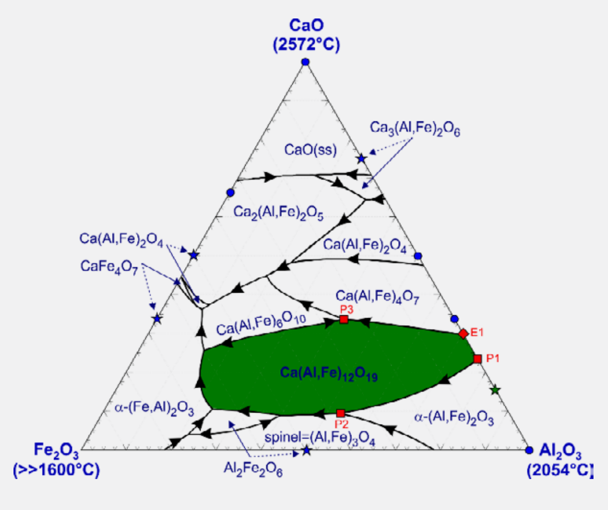

Fig. 2

The concentration triangle $CaO–Al_2O_3–Fe_2O_3$, calculated with FactSage 8.1. Compositions of congruently melting binary compounds are marked by a circle, an asterisk marks a peritectically melting compound. The eutectic and peritectic points shown in red have the following positions: E1: 1754°C, 29.7% CaO; P1: 1833°C, 23.4% CaO; P2: 1724°C, 9.4% CaO; P3: 1560°C, 33.6% CaO. Note that compositions in the Fe_2O_3-rich corner decompose partially under the formation of Fe^{2+} (e.g., the spinel phase) at the bottom.

References

[1] Y. Kajiwara, K. Harii, S. Takahashi, J. Ohe, K. Uchida, M. Mizuguchi, H. Umezawa, H. Kawai, K. Ando, K. Takanashi, S. Maekawa, E. Saitoh, Nature, 464 (2010) 262-266.

[2] A.V. Chumak, V.I. Vasyuchka, A.A. Serga, B. Hillebrands, Nature Physics, 11 (2015) 453-461.

[3] H. Dötsch, D. Mateika, P. Röschmann, W. Tolksdorf, Materials Research Bulletin, 18 (1983) 1209-1216.

[4] D. Mateika, R. Laurien, Journal of Crystal Growth, 52 (1981) 566-572.

[5] D. Klimm, B. Szczefanowicz, N. Wolff, M. Bickermann, J Therm Anal Calorim, in press, DOI: 10.1007/s10973-021-11050-4, (2021).

[6] C. Guguschev, C. Richter, M. Brützam, K. Dadzis, C. Hirschle, T.M. Gesing, M. Schulze, A. Kwasniewski, J. Schreuer, D.G. Schlom, Crystal Growth & Design, 22 (2022) 2557-2568.

Transfer Printable Single-Crystalline Coupons for III-V on Si Integration

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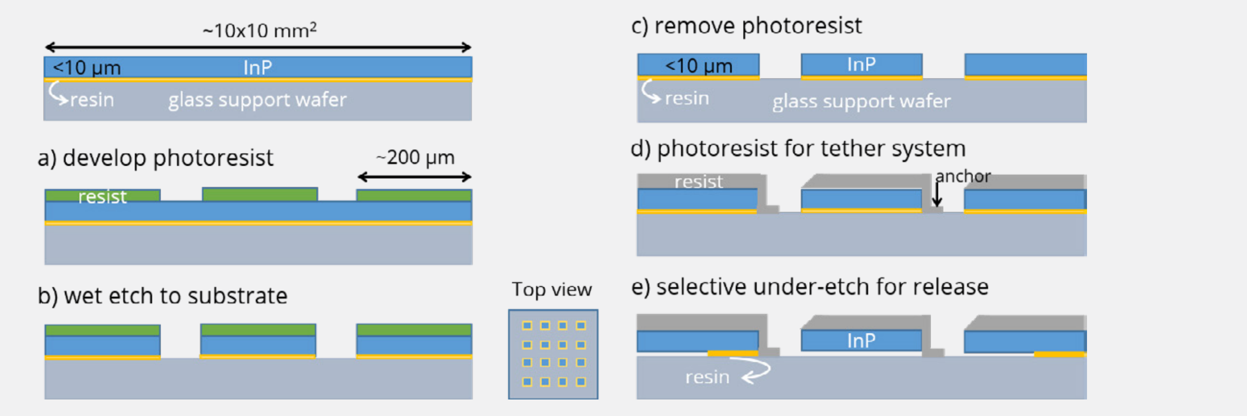
The next-generation internet (6G) requires highly functional devices that e.g. realize frequencies in the THz range for higher data rates and lower latencies. Those requirements exceed the physical limits of established CMOS technologies based on silicon (Si). Hence, there is demand for other semiconductor materials with superior electronic and optical properties that complement Si. One of the key candidates is the III-V compound semiconductor, indium phosphide (InP). Due to its high electron mobility and direct band gap, InP-based devices allow access to frequencies >100 GHz and operate at the optical fibre compatible wavelength of 1.55 µm [1].

With the perspective of leveraging the advantages of Si-based CMOS technology and III-V semiconductors, hetero-integration of III-V materials on Si is of great interest. However, existing integration approaches entail certain disadvantages: (i) high dislocation densities due to the lattice mismatch of InP and Si for integration via *hetero-epitaxial growth* [2]; (ii)limited integration density and the requirement of accurate alignment for *flip-chip* integration; and (iii) high process-related losses of Si and III-V material as well as thermal stress and low thermal conductivity of adhesive layers degrading device performance for *wafer/die bonding* technologies [3].

Another promising approach for III-V-on-Si is *micro-transfer-printing* (µTP) that involves pick up and transfer of µm-small chips from a source substrate to a target substrate with high alignment accuracy by using an elastomeric stamp. Advantages of µTP are high integration densities and efficient material use. The technique was already implemented for III-V-on-Si photonic integrated circuits by transfer of epitaxial III-V layers [4]. But, using sacrificial interlayers for release and adhesives for bonding leads to transfer issues and low operation temperature for the devices, respectively.

We pursue a new approach to hetero-integration of InP on Si that aims at the transfer and adhesive-free bonding of single-crystalline InP coupons onto Si via µTP. This will be achieved by obtaining crystalline coupons with a thickness of $d \leq 10$ µm and two polished surfaces that achieve the low roughness i.a. needed for effective adhesive-free bonding. If the high structural quality of the single-crystalline InP source material can be maintained, this process will provide high quality templates for subsequent epitaxial growth. Towards this goal, we developed a sophisticated micro-preparation process in cooperation with the Leibniz Institute for High Performance Microelectronics IHP, which we filed as a patent [5]. Starting from 4-inch single crystals with homogeneous, low dislocation density of $2{\times}10^3$ cm^{-2} grown at IKZ [6], thinned InP dies were obtained by sawing, grinding and an optimized two-step chemical mechanical polishing (CMP). In order to produce µm-sized transfer-printable coupons, the InP dies were micro structured by lithography assisted patterning and wet etching (Fig. 1a–c).

Fig. 1
Micro structuring for transfer printable single-crystalline InP coupons.



For the transfer, the InP coupons need to be encapsulated with a photoresist with local openings to access the resin fixing layer, which is then under-etched, leaving the free standing InP coupons anchored to the glass substrate by tethers (Fig. 1d– e). The coupons can then be picked up with a stamp and transferred to the target wafer. Main innovation of this process is the resin which serves as low stress fixing layer for CMP as well as sacrificial layer for later release.

The optimized CMP process with abrasive-free final polishing yielded InP platelets of the desired thickness below 10 µm with low thickness deviation < 1 µm and excellent surface roughness of $S_q \approx 0.3$ nm (Fig. 2a-d). This value even meets the requirements for adhesive-free bonding ($S_q \leq 2$ nm) and subsequent epitaxial growth ($S_q \leq 0.5$ nm). X-ray rocking curve mapping provides accurate spatial maps of lattice deformations in the material that may be a consequence of the mechanical processing. Rocking curve widths mappings of the 004 reflection of a (001) sample before and after thinning are homogeneous and below 25 arcsec in the major part of the sample area (Fig. 3a-b). However, spots of higher FWHM on the thinned sample indicate damaged areas. These can also be identified by optical microscopy (Fig. 3c), and are attributed to bubbles in the fixing layer. The local damage can be avoided in future by sample fixation under vacuum. Overall no signs of systematic crystal quality deterioration in the product platelets compared to bulk samples have been detected. For non-destructive determination of dislocation densities in µm-thin samples, we envision to make use of imaging techniques like cathodoluminescence or electron channelling contrast in the future.

In summary, the feasibility of µm-thin InP platelet fabrication was demonstrated. Final platelets meet the prerequisites of low and uniform thickness, high planarity, low roughness and little crystal quality deterioration. Furthermore, first InP platelets could successfully be patterned to 100–400 µm-sized coupons using optical lithography and wet etching. It is now possible to take the next steps towards hetero-integration on Si via µTP – a technique that will likely outperform hetero-epitaxial growth in crystal quality, and heterogeneous integration methods in device performance and integration density.

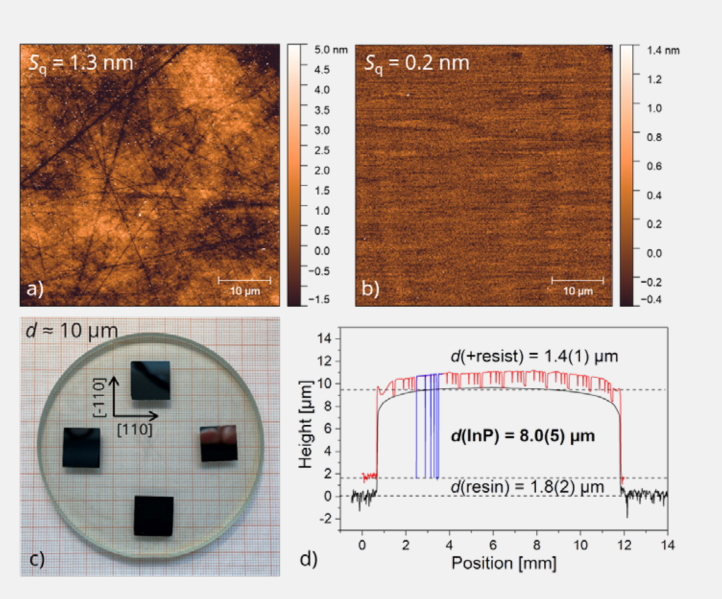


Fig. 2
AFM scanning images of a surface after CMP with
a) alumina abrasive and
b) abrasive-free solution;
c) final thinned and polished InP platelets mounted on a glass substrate;
d) height profiles of InP platelet with resin (black), with additional developed resist (red) and after wet etching (blue).

References

[1] J. C. Rode, et al. *IEEE Trans. Electron Devices* 2015, 62, 2779–2785.

[2] Q. Li, K. M. Lau *Prog. Cryst. Growth Charact. Mater.* 2017, 63, 105–120.

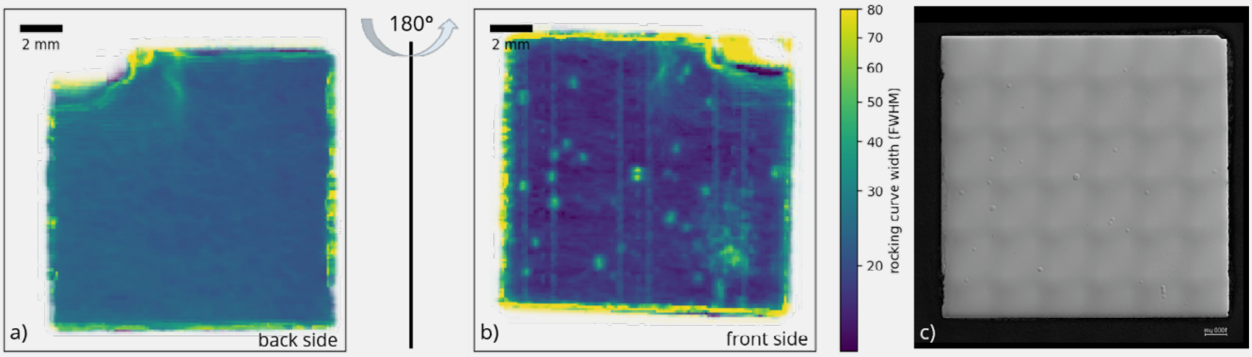
[3] X. Guo, A. He, Y. Su *J. Semicond.* 2019, 40, 101304.

[4] J. Zhang, et al. *APL Photonics* 2019, 4, 110803.

[5] IKZ-IHP Patent filed - DE 10 2022 100 661.1

[6] K. Giziewiczet, L. Smejkalova, St. Eichler, U. Juda, M. Pietsch, O. Root, D. Souptel, K. Stolze, B. Weinert, Ch. Frank-Rotsch 5*1st Annual Meeting of the German Association of Crystal Growth (DKT2021), 2021,* Berlin.

Fig. 3
Mapped rocking curve FWHM of <001> sample
a) before and b) after thinning, the sample was flipped during the process, the missing corner in both maps attributes to a grain of different orientation; and c) micrograph of an InP platelet, shadows are artefacts from stitching.



[211] and [110] grown Germanium crystals for dislocation tuning

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Germanium (Ge) single crystals are used in several modern technological applications, such as infrared optics, substrates for epitaxy, and detectors for X-rays or gamma-rays. Further, the small bandgap, the high charge carrier mobility and also its availability with very high purity are appealing properties that make Ge more suitable than silicon (Si) in many electronic devices as well, since integrated circuits and transistors of Si have faced physical limitations due to their fundamental properties. For most of the applications it is required that the Ge crystal should have a high degree of crystalline perfection with a minimum dislocation density, besides meeting many other important requirements. Hence, dislocation structure analysis and its control in Ge bulk single crystals grown by the Czochralski (Cz) method are important.

The standard Ge technology currently employed revolves around the crystals grown in [100] direction. We have made preliminary investigations of the impact of the growth direction on the dislocation structure of Ge crystals and correlated that to the charge carrier lifetime. For the purpose of this report, we discuss the results of Ge crystals grown in [211] and [110] and more details of this work can be found in [1, 2].

The central technology controlling the dislocation density in [100] Cz-Ge crystal is the Dash neck. This technique relies on the grow-out of dislocations due to the {111} dislocation glide planes being non-parallel to the growth direction. Therefore, we have studied crystals grown in growth directions parallel to dislocation glide planes. There are an infinite number of such directions, but the [110] and [211] directions are the ones with the lowest Miller indices, which have special geometric significance for dislocation propagation. In contrast to [110] – which is parallel to two glide planes – [211] is the lowest index direction which is parallel to only one glide plane. Hence, one would expect that the dislocations can be restricted to this single glide plane if a Dash neck procedure is conducted in the [211] direction. Further analysis [1] – reveals that the dislocation lines get restricted to two remaining dislocation line directions, namely [110] and [101].

For this investigation, Ge crystals were grown in [211] and [110] direction in Argon gas atmosphere. Seed crystals oriented in [211] and [110] direction (deviation < 1°) have been fabricated from carefully selected Ge single crystals. The crystals were grown with a long Dash neck with higher pulling rates between 110 mm/h and 180 mm/h. Thereafter, the crystal shoulder was realized by reducing the pulling rate gradually to 60 mm/h, which was kept constant throughout the entire remaining crystal growth process to have the crystal with constant diameter of approximately 45 mm. Proper care has been taken to minimize the contaminations in every stage including zone-refined starting material, which was etched, cleaned, and loaded in a graphite crucible that is coated with a pyrolytic carbon. The final crystal showed the intrinsic charge carrier density at room temperature, throughout the entire crystal, determined by the Van der Pauw method. One such [211] crystal is shown in Fig.1 and it has a faceted, trapezoid, non-rotational symmetric shape. (111) wafers (longitudinal crystal section) were cut and chemo-mechanically polished, for the purpose of white beam X-ray topography, etch pit density, and charge carrier lifetime analysis.

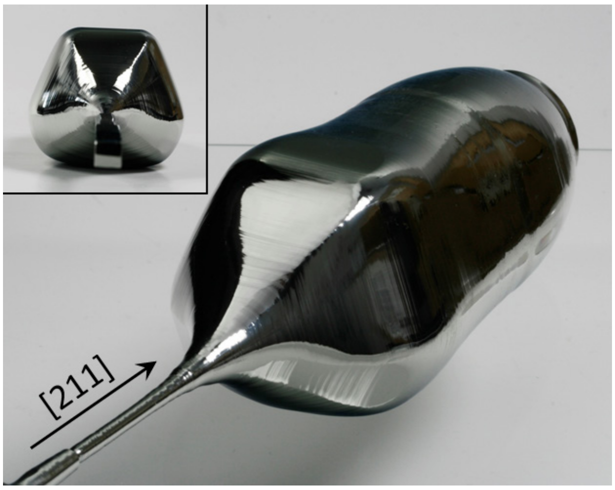

Fig.1
Nicely facetted [211] Ge crystal (45 mm diameter) grown by the Cz technique. The inset figure shows the top view of the crystal, revealing a trapezoid, non-rotational symmetric crystal shape.

The white beam X-ray topography measurements for the dislocation investigation were conducted in transmission geometry at Karlsruhe Research Accelerator (KARA), at the Karlsruhe Institute of Technology (KIT) light source. A 311 topograph of the sample taken shortly after the Dash neck in the crystal reveals that most dislocation lines are aligned to the [110] and [101] directions. The dislocation density in the selected area was estimated as 280 cm^{-2}. X-ray topography data enabled us to conduct a Burgers vector analysis for selected dislocation lines, studying their visibility in the 133, 3-13, 220, 202, 24-2, 2-24, 313, and 331 reflexes. All dislocation turned out to be screw dislocation, which is the preferential dislocation type, having the least impact on the electronic properties of the material. Hence, we could show that on top of the dislocation line orientation selection, a dislocation type selection took place [1].

For reference and larger statistics of dislocation densities, an etch pit density analysis was conducted. The polished wafers were etched in a 1:1 mixture of 40% hydrofluoric acid and 50 g CrO_3 in 100 ml water for 45 min, which preferentially etches the {111} facets in Ge, and hence produces tetrahedral etch pits at dislocation cores on the (111) sample surface.

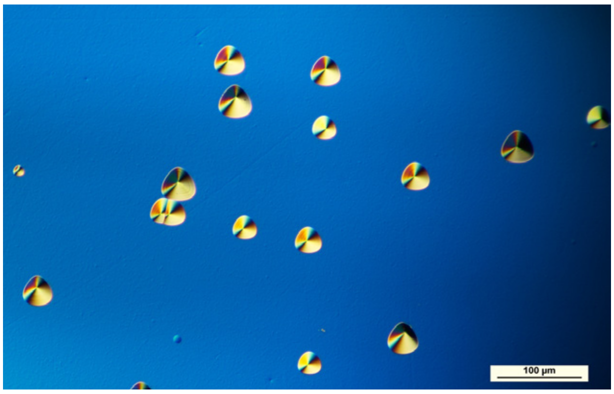

Fig. 2
Tetrahedral-shaped etch pits observed on the [110] crystal by the differential interference contrast optical microscopy (DIC).

A single micrograph (DIC) of the etched surface of the top part of the [110] crystal is depicted in Fig. 2. It is to be mentioned that the etch pits on both the [110] and [211] crystals are identical in shape and showed tetrahedral morphology. The dislocation structure of the grown [211] Ge crystals was analyzed in an etched longitudinal section with (111)-orientation by optical microscopy with differential interference contrast (DIC). The micrographs of these sections were stitched together to investigate the macroscopic distribution of etch pits as can be seen in Fig. 3a. The dislocation density gradually increases from close to dislocation-free shortly after the Dash neck, to dislocation densities above 10^4 cm^{-2} close to the crystal tail. The etch pit density was correlated with the charge carrier lifetime determined by microwave-detected photo-conductance decay, presented in Fig. 3b. The charge carrier lifetime is above 600 µs for most of the crystal and only decays significantly at a dislocation density threshold of $3\cdot10^4$ cm^{-2}.

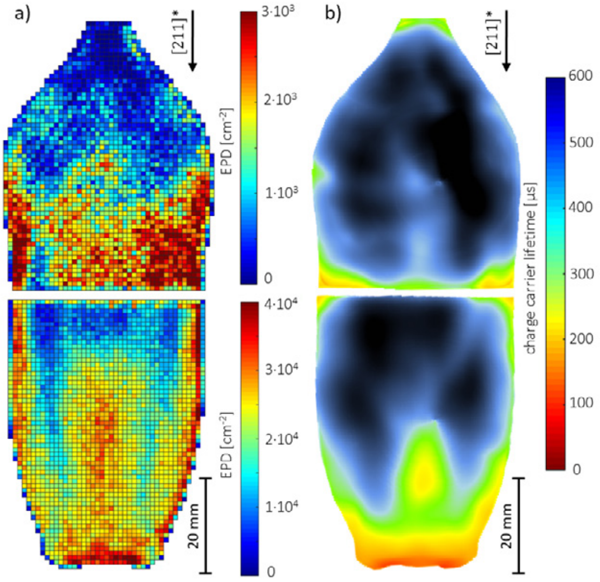

Fig. 3
(a) Etch pit density map and (b) charge carrier lifetime of the [211] crystal (Figures reprinted from Ref. 2).

We conclude that a successful Dash necking procedure in [211] Cz-Ge crystals leads to a dislocation line and dislocation type selection, which was shown to lead to a charge carrier lifetime of 600 µs with a tolerance to dislocations up to a dislocation density of $3\cdot10^4$ cm^{-2}.

Acknowledgement

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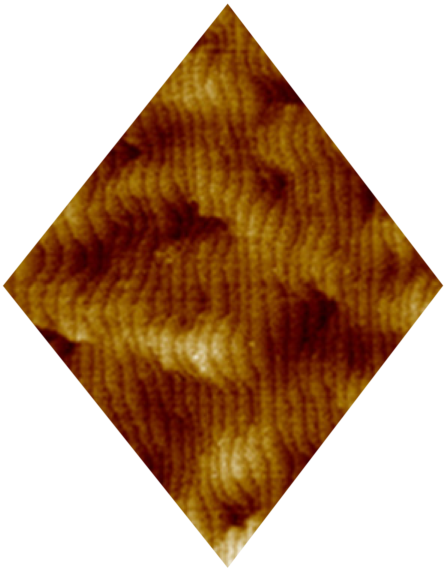
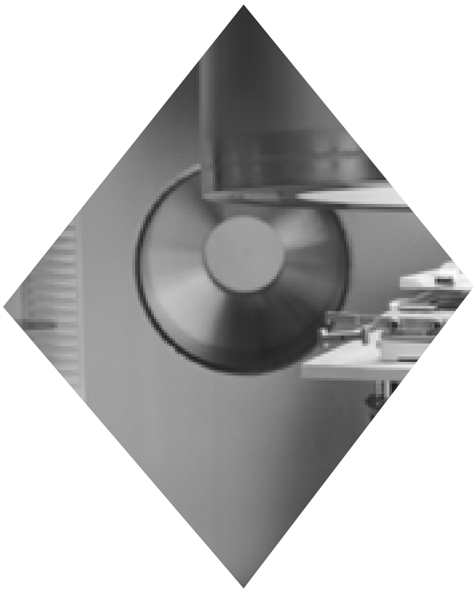
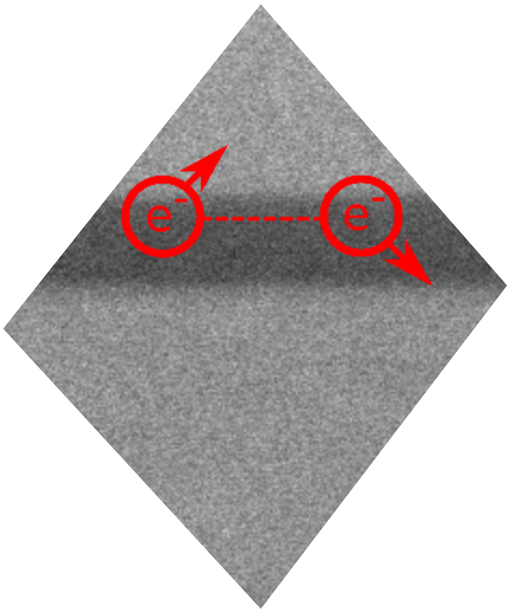
References

[1] K.-P. Gradwohl, M. Roder, A.N. Danilewsky, R.R. Sumathi, CrystEngComm 23.23 (2021): 4116-4124.

[2] K.-P. Gradwohl, U. Juda, and R. R. Sumathi, Journal of Crystal Growth 573 (2021): 126285.







Nanostructures & Layers

MOVPE of (100) β-Ga_2O_3 for vertical power devices – Challenges to the Epitaxy Process

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Due to its wide bandgap of about 4.85 eV beta gallium oxide (β-Ga_2O_3) is considered as a promising candidate as base material for high power converters and solar-blind UV photodetectors. High-power transistors based on β-Ga_2O_3 are predicted to outperform the current SiC- and GaN-based technology due to three times higher theoretically electrical breakdown field (8.0 MV/cm). Therefore, β-Ga_2O_3 is attractive for the future development of power conversion systems, contributing to lowering the overall CO_2 production and the power loss. The potential of β-Ga_2O_3 can be best exploited in β-Ga_2O_3-based high power transistors using a vertical device architecture. Such device structure will benefit from a low on-resistance at a given breakdown voltage combined with less power losses during switching operation. However, the vertical device architecture leads to new requirements within the whole process chain, from bulk crystal growth over epitaxy to device development. Focusing on the epitaxy, high-quality homoepitaxial layers with a low doping level ($\leq 5\times10^{16}$ cm^{-3}) and a thickness of several μm are the main requirements to achieve suitable drift zone layers for the later device.

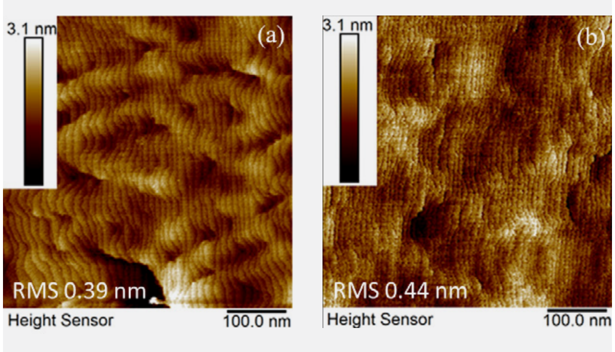

Fig. 1
AFM images of homoepitaxial (100) β-Ga_2O_3 thin films grown by applying the developed growth condition with a doping level at 1×10^{18} cm^{-3} and different thickness: (a) 0.3 μm and (b) 3 μm.

The β-Ga_2O_3 bulk crystal is grown by the Czochralski method at IKZ [1], and (100) oriented β-Ga_2O_3 wafers were prepared at CrysTec GmbH in Berlin. The (100) orientation is our main research interest since it is a cleavage plane and exhibits the lowest surface energy. All (100) oriented wafers were prepared with an offcut angle of 4° towards $[00\bar{1}]$ which results in a regular step-and-terrace surface structure with a terrace width of about 8.5 nm. The usage of such vicinal surfaces avoids the formation of twin lamellae during the epitaxial growth process and lead to low defect densities in the layers.

Our previous works identified the importance of substrate miscut [2] and the influence of growth parameters on the effective diffusion length of the adatoms [3] to maintain a step-flow morphology of the grown layer and ensure the quality of the layers. To achieve the requirements of the vertical device now, one of the key challenges is to grow thick layers up to 3 μm while maintaining step-flow morphology, which has not been demonstrated yet on (100) orientation. In our recent work [4], we found out that by increasing the Ga flux and adjusting the O_2/Ga ratio down to 300 (before 1200, while fixing other growth parameters), the desired step-flow morphology can be maintained up to 3 μm (see Figure 1). With this we increased our maximum layer thickness by a factor of 10 compared to our previous results. A "Ga-adlayer" is considered as a possible mechanism for the successful control of the growth mode. We believe that with an excessive amount of Ga precursor on the surface, a metallic-adlayer forms as an alternative diffusion channel. In addition the Ehrlich–Schwöbel Barrier (ESB) on the step edges is screened, which largely promotes adatom diffusion rates and growth morphology planarization. A similar mechanism is found for the system of GaN and GaAs.

With this new growth parameter the realization of thick epitaxial β-Ga_2O_3 layers with an electron Hall mobility of about 144 $cm^2\ Vs^{-1}$ at an electron concentration ~of 1.5 × 10^{17} cm^{-3} are possible as shown in Figure 2. This value of the electron mobility is comparable with the highest value reported by us (about 150 $cm^2\ Vs^{-1}$ at ~ 1.4 × 10^{17} cm^{-3}) for β-Ga_2O_3 thin films grown on offcut (100) β-Ga_2O_3 substrates with a thickness of 300 nm. The high measured mobility also implies a low density of structural defects in the layers which implies that there is no trade-off on electrical properties while pursuing a thicker layer. Of course, a lower doping level down to 5×10^{16} cm^{-3} is the next milestone we are working on now.

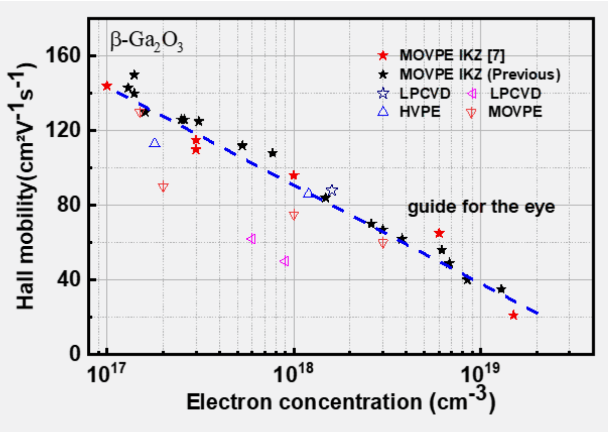

Fig. 2
The electron Hall mobility (red asterisk) of β-Ga_2O_3 films grown on (100) β-Ga_2O_3 substrate as a function of electron concentration [4]. Other symbols show results from the literature.

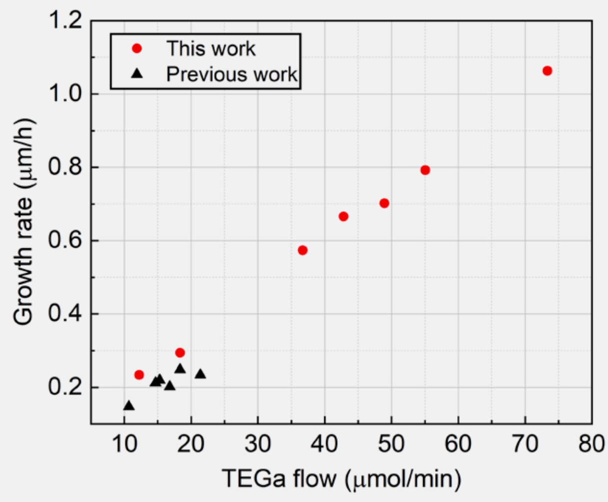

Fig. 3
The growth rate of (100) β-Ga_2O_3 thin films as the function of the TEGa flow to ensure a constant O_2/Ga ratio close to 300, the oxygen flow is increased accordingly. Red circles represent results for films grown at the growth condition used in [4], and the black triangles represent our previous work.

By keeping a low O_2/Ga ratio at 300, the growth process with the step-flow morphology can be up-scaled proportionally with a growth rate increasing above 1.0 µm/h as shown in Figure 3. A high growth rate is desirable for industry application, and lowers the incoperation of background impurities.

Acknowledgments

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References

[1] Galazka, Z., Ganschow, S., Seyidov, P., Irmscher, K., Pietsch, M., Chou, T.S., Anooz, S., Grueneberg, R., Popp, A., Dittmar, A., Kwasniewski, A., Suendermann, M., Klimm, D., Straubinger, T., Schroeder, T. and Bickermann, M. "Two inch diameter, highly conducting bulk b-Ga2O3 single crystals grown by the Czochralski method". Appl. Phys. Lett., 120, 152101. 2022. (Editors Pick)

[2] S. Bin Anooz, R. Grüneberg, C. Wouters, R. Schewski, M. Albrecht, A. Fiedler, K. Irmscher, Z. Galazka, W. Miller, G. Wagner, J. Schwarzkopf, and A. Popp, Appl. Phys. Lett. **116**, 182106 (2020).

[3] S. Bin Anooz, R. Grüneberg, T.S. Chou, A. Fiedler, K. Irmscher, C. Wouters, R. Schewski, M. Albrecht, Z. Galazka, W. Miller, J. Schwarzkopf, and A. Popp, J. Phys. D. Appl. Phys. **54**, 034003 (2021).

[4] T.-S. Chou, P. Seyidov, S. Bin Anooz, R. Grüneberg, T. Thi Thuy Vi, K. Irmscher, M. Albrecht, Z. Galazka, J. Schwarzkopf, and A. Popp, AIP Adv. **11**, 115323 (2021)

Towards the development of novel 2D-cristalline materials via Layer Transfer

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Crystalline heterostructures and material interfaces constitute an important route to engineer functional materials. In this respect, layer transfer establishes a new paradigm since it allows the combination of crystalline materials irrespective of thermodynamic, kinetic or geometrical constraints limiting traditional hetero-epitaxial growth methods. Thus, layer transfer expands the possibilities of engineering material properties. Specifically, with 2D-van der Waals materials, such as graphene or transition metal di-chalcogenides, it has been demonstrated that by mere control of the stacking-order and orientation of 2D-materials emergent properties and strongly correlated electronic phases can be realized [1, 2]. Examples include superconductivity, Mott-insulating phases, as well as exciton condensates. The respective heterostructures, for example twisted stacks, can often only be realized by layer transfer and are out of reach of traditional epitaxial methods. This is why layer transfer has been established as "bottom-up" method for the fabrication of novel "2D goes 3D" crystalline materials.

Aside from fundamental research, layer transfer may also contribute to technological applications. We note that high-performance optoelectronics combine specific device-functionalities with optimal performance. In order to achieve this, it is required to combine modules based on different crystalline materials, for example the integration of optical components based on III-V semiconductors on CMOS-chips. With "micro-transfer printing", a method related to layer transfer is being established on industrial scale. IKZ is seeking for impact with respect to materials development in basic research, as well as in the field of applications. With the installation of a home-built layer transfer station, IKZ develops its own transfer technology.

The placement of nanometer thin films with high spatial accuracy is best done with the help of a micromanipulator. We have set-up a 6-axis micro-robot inside a high vacuum chamber (Fig 1:) to conduct layer transfer in inert gas atmosphere at variable pressure to minimize adsorption of water and other contaminations. In addition, we are designing functional Polydimethylsiloxane (PDMS)-stamps to allow for robust and reliable transfer of 2D-materials.


photo: Simon Eichmann

Fig. 1
Layer Transfer Station

In the long run, the layer transfer station should encompass the complete process from in-situ epitaxy of 2D-crystalline materials, including release and pick & place process.

Epitaxial films of non-van der Waals materials are usually firmly bonded onto the substrate on which they are grown. In order to release thin films from the substrate different approaches can be pursued. We work with oxide perovskites and adopt the concept of water-soluble sacrificial layer [3]. We utilize pulsed layer deposition (PLD) for its flexibility in producing a large range of different epitaxial oxide materials. So far, we have reproduced published results employing $Sr_3Al_2O_6$ (SAO) as sacrificial layer and testing various perovskites as capping, or functional, layer. This includes $SrTiO_3$ (STO), $SrRuO_3$ (SRO), $LaAlO_3$, and (K,Na)NbO_3. For the SAO/STO heterostructure, we systematically varied the oxygen pressure amd growth temperature and optimized layer thickness to achieve good crystalline quality and surface roughness for sacrificial layer and functional film.

We determined as best growth conditions a substrate temperature of 700°C for both, SAO and STO growth. Interestingly, to avoid parasitic phases for SAO, the oxygen pressure within the chamber should be kept below 10^{-4} mbar. Most likely this is due to the influence of background pressure on the stoichiometric composition of the plume. In contrast, STO requires higher oxygen pressure (~ 10^{-2}mbar) to minimize oxygen vacancies. Detailed fitting of the XRD data (not shown) reveals that the SAO layer is relaxed for film thickness larger than 20nm which is attributed to the noticeable lattice mismatch between the SAO and the STO of about 1.4%.

After PLD growth, the epitaxial heterostructure is immersed in water to release the functional film while being supported by a soft stamp made of PDMS. The PDMS-stamps functions as carrier support for the film and allows easy handling. While the dissolution of the sacrificial layer is conducted manually, we employ the layer transfer station for the final transfer onto the target substrate. Aside from alignment in the few micrometers regime, we can also control the pressure and temperature with which the transfer process is conducted. Figure 2 shows an optical micrograph of a transferred film. The overall transfer efficiency is high (> 90%), yet often the transferred film displays cracks and wrinkles. This requires further improvements.

As an example, we show the transfer of a freestanding 20 nm $SrRuO_3$ thin film on a Si substrate. In the first step, the sacrificial layer SAO is grown on the $SrTiO_3$ substrate, the occurrence of thickness oscillation nearby the SAO film peak in the XRD data in Fig. 3 (red curve) verifies the high structural quality of the SAO film. Subsequently, a 20 nm thin $SrRuO_3$ film was epitaxially grown on the SAO/STO heterostructure (blue curve) and successfully transferred to a Si wafer (green curve).

These results have been obtained within two Master Thesis.

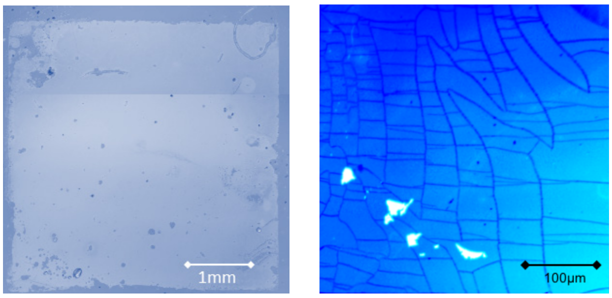

Fig. 2

Transferred $SrTiO_3$ *thin films (10nm) on* SiO_2*/Si-wafer. While the transfer efficiency is high, the transferred films still display cracks.*

In parallel with the set-up of the transfer station we have successfully acquired in 2021 a research project from the German Research Foundation (DFG) “Nanotwist: twisted epitaxial perovskite heterostructures”. This project started in November 2021 with a PhD student and with the aim to investigate the effect of shear strain on the properties of perovskites at artificial twist boundaries. With repeated thin film layer transfer we will form twist boundaries within few nanometers from the surface, allowing the use of AFM-based techniques and the investigation of these interfaces in unprecedented detail.

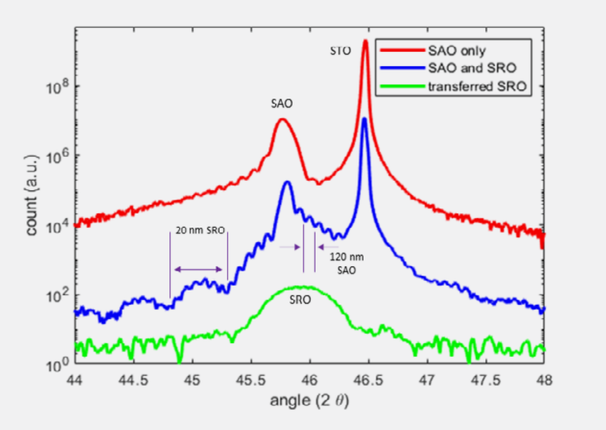

Fig. 3

XRD-patterns of sacrificial layer ($SrAl_2O_3$) *on* $SrTiO_3$*-substrate without capping layer (red), sacrificial layer and* $SrRuO_3$ *capping layer (blue), and transferred heterostructure SrRuO3-Film on* SiO_2*/Si-substrate (green)*

References

[1] Cao, Yuan, Valla Fatemi, Shiang Fang, Kenji Watanabe, Takashi Taniguchi, Efthimios Kaxiras, and Pablo Jarillo-Herrero. “Unconventional superconductivity in magic-angle graphene superlattices.” *Nature* 556, no. 7699 (2018): 43-50.

[2] A. Ciarrocchi, F. Tagarelli, A. Avsar, A. Kis; “Excitonic devices with van der Waals heterostructures: valleytronics meets twistronics.” *Nature Reviews Materials* (2022): 1-16.

[3] Lu, Di, David J. Baek, Seung Sae Hong, Lena F. Kourkoutis, Yasuyuki Hikita, and Harold Y. Hwang. “Synthesis of freestanding single-crystal perovskite films and heterostructures by etching of sacrificial water-soluble layers.” *Nature materials* 15, no. 12 (2016): 1255-1260.

Controlling and ensuring neutral spin environments for future applications in Si heterostructures

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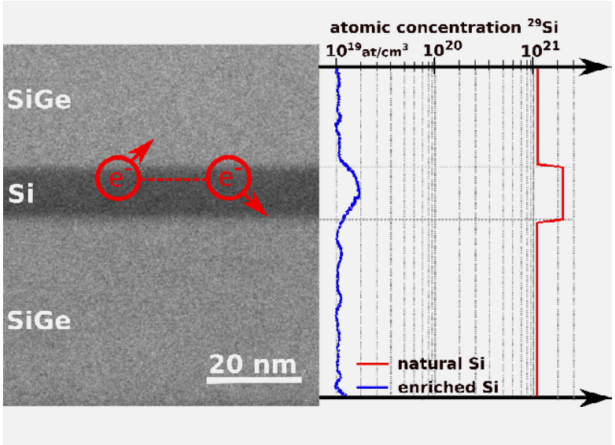
New challenges for crystallography and crystal growth arise from the constantly increasing demands on modern computing and communication technologies. This greatly affects the research and development of crystalline nanomaterials, as Moore's Law runs the risk of coming to an end due to the physical limits of miniaturisation. In addition, there is strong interest in integrating photonic emitters into silicon, as the indirect band prevents the optical activity of the material itself. To address these challenges at the nanometre scale, new ideas need to be developed and commonly used knowledge re-evaluated.

Two of these challenges are being addressed by the IKZ and project partners: On the one hand, the design of Si-Ge heterostructures for semiconductor quantum computers and, on the other hand, the embedding of optically active quantum dots in silicon-on-insulator systems (SOI) are being investigated. The first topic is worked on together with the Leibniz Institute for High Performance Microelectronics (IHP) in Frankfurt/Oder and partners at the RWTH Aachen, the Institut für Quanteninformation (IQI) and the Institut für Halbleitertechnik (IHT). The IKZ is conducting joint research on the latter topic with the Max-Planck-Institut für Quantenoptik (MPQ) in Garching and the Munich Center for Quantum Science and Technology (MCQST) at the Ludwig-Maximilians-Universität München.



Spin qubits in semiconductor materials such as Si-Ge are promising candidates for basic functional elements to realise the universal quantum computer (QC). In recent years, various concepts have been developed to achieve qubits, the computational units of QCs, from physical systems such as trapped ions, superconducting circuits or nitrogen vacancies in diamond. Yet only systems based on single electrons in semiconductors can be scaled to the necessary very large number of qubits and also have the advantage of being compatible with established fabrication technologies such as Si-CMOS manufacturing [1]. Two single electrons must be captured, entangled, modified and analysed to serve as a qubit. This is realised by SiGe/Si/SiGe heterostructures in which the electrons are trapped in the buried and elastically deformed Si layer (Fig. 1, left). This electron system is very sensitive to external disturbances, which is why it must be shielded against undesired external electric and magnetic fields as well as thermal influences. But not only external factors can affect the entanglement of the enclosed electrons. Internal disturbances such as impurities, defects or interface steps can also impact the electronic system. It has been shown that even a few atomic steps on the SiGe/Si interface can result in an inhomogeneity that causes the controlled qubit to collapse [2]. Impurities with odd nuclear spin can also lead to decoherence of the electron, as they bring with them a random local magnetic field. Unfortunately, natural Si itself contains an isotopic species with odd nuclear spin: ^{29}Si. For the development of Si-based semiconducting QCs, starting materials are thus attractive that are depleted in ^{29}Si or, in the best case, enriched with ^{28}Si.

Fig. 1
SiGe heterostructures for semiconductor QCs. Left: A TEM image of the material system. In a strained Si layer of less than 10 nm thickness, two electrons are trapped and entangled with each other (added as red symbols). Right: To maintain the electron spins, the concentration of ^{29}Si in the material must be minimised. The SIMS measurement shows a concentration of max. 2×10^{19} at/cm^3 in the enriched Si layer (blue data). For natural Si, values two orders of magnitude larger can be expected (red line).

Very similar problems arise when integrating quantum optical emitters into SOI systems. Individual dopants can be used in Si to create optically active quantum dots [3]. Since these have to be coupled with external electric and magnetic fields and the coherence of the emitters is strictly limited by this coupling, any internal inhomogeneity can affect the system. And again, the decoherence even originates from the isotope ^{29}Si present in natural Si.

The challenges for crystallography and crystal growth in these two examples are manifest: First, growth should be done with isotope-depleted or even -enriched materials, and isotopic purity should be maintained during growth and further processing. Second, the nanoscopic layers must be deposited with a quality and accuracy rarely achieved. Since subsequent etching or grinding of these fragile ultrathin layers is difficult, the growth process itself must ensure perfect layers in a reproducible and scalable manner.

The growth of the isotope-enriched ^{28}Si layers is carried out by molecular beam epitaxy (MBE). For the QC research, SiGe substrates produced at IHP by chemical vapour deposition are applied. A SOI seed substrate is used as the substrate for ^{28}Si on SOI to build quantum optical emitter. Both substrate types have to be wet-chemically cleaned to ensure a perfect interface with a surface roughness of less than 1 nm. The growth process takes place under ultra-high vacuum. A target material of solid ^{28}Si serves as the solid-state source. The material is produced by the research group “FZ-Si” at the IKZ and has an isotopic purity of 99.99% ^{28}Si [4]. The research task is to maintain this purity during the MBE growth process. For characterisation, the grown ^{28}Si films were analysed by secondary ion mass spectrometry (SIMS). The SIMS measurements show a small amount of parasitic ^{29}Si in the grown films (Fig. 1, right). The concentration of ^{29}Si is about 1×10^{19} - 2×10^{19} at/cm. This corresponds to a purity of 99.96%-99.98% ^{28}Si. Thus, it is possible to almost completely transfer the isotopic purity of an enriched solid source to thin films grown by MBE.

The second challenge is to produce atomically perfect surfaces and interfaces. For this, transmission electron microscopy (TEM), atomic force microscopy (AFM) and X-ray diffraction (XRD) methods can be used for characterisation. All techniques show surface and interface roughness of less than 1 nm. This is a very fine value. Nevertheless, it is not perfect at the atomic level. To reduce the surface and interface roughness even further is a current challenge. For this purpose, we vary the growth parameters to empirically determine perfect conditions. Yet we are also investigating the system on a more fundamental basis.

Physical forces act on surfaces and interfaces that can cause roughness or even instability. By taking into account the (atomic) interactions, e.g. the Van der Waal forces, and the external influences, e.g. gravity, the effective force can be calculated. In a research article, we have shown that the results of these calculations can be used to modify an Au surface on Si [5]. Depending on the effective force, the growth parameters and the energy introduced into the system, a surface can be roughened or even made to collapse. A current challenge is to transfer the results of the Si/Au system to SiGe/Si resp. SOI and to reverse the effect in order to produce atomically smooth layers. To do this, the forces acting on and off the surface have to be balanced: a challenging task that will require a fair amount of theoretical and empirical research in the future.

The further miniaturisation of modern technology challenges crystallography to grow thin crystalline films with unprecedented perfection. The design of Si-Ge heterostructures for semiconductor QCs and the embedding of optically active quantum dots in SOI systems require the maintenance of isotopic purity during growth and the fabrication of atomically perfect nanoscopic layers. We have shown that the isotopic purity of an enriched solid source can be transferred to thin films grown by MBE. However, the production of perfectly smooth layers is still a challenge and a task for further research and development at the IKZ.

References

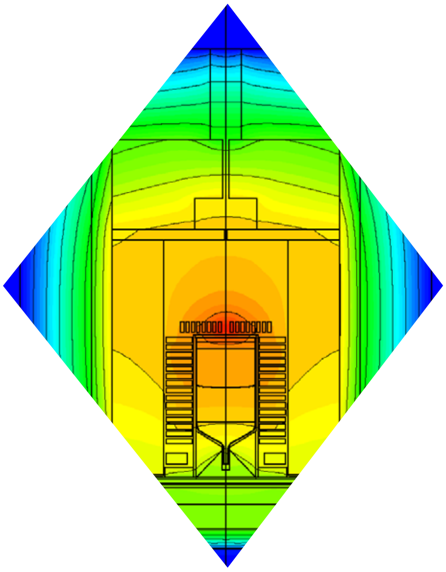
[1] A. Hollmann, T. Struck, V. Langrock, A. Schmidbauer, F. Schauer, K. Sawano, H. Riemann, N.V. Abrosimov, D. Bougeard, L.R. Schreiber, *Large and tunable valley splitting in Si/SiGe quantum dots*, Phys. Rev. Applied 13 (**2020**) 034068

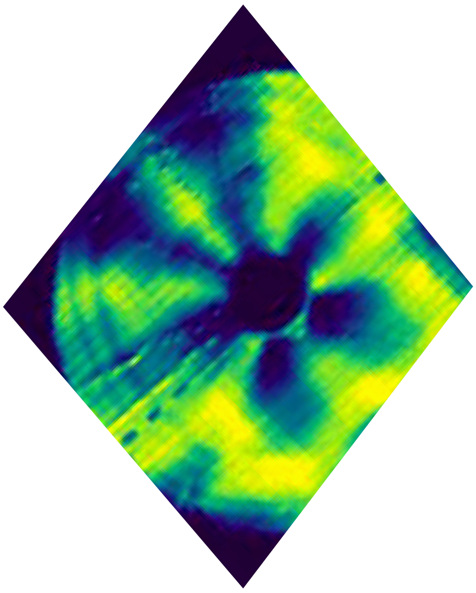
[2] M. Friesen, S. Chutia, C. Tahan, and S. N. Coppersmith, *Valley splitting theory of SiGe/Si/SiGe quantum wells*, Physical Review B - Condensed Matter and Materials Physics, 75 (**2007**) 1–12.

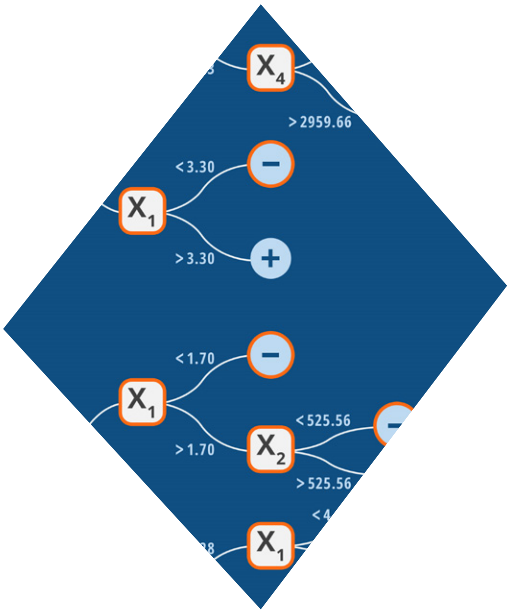
[3] A. Gritsch, L. Weiss, J. Früh, S. Rinner, A. Reiserer *Narrow optical transition in erbium-implanted silicon waveguides* arXiv preprint arXiv:2108.05120 (**2021**)

[4] N. V. Abrosimov, D. G. Aref’ev, P. Becker, H. Bettin, A. D. Bulanov, M. F. Churbanov, S. V. Filimonov, A. V. Gavva, O. N. Godisov, A. V. Gusev *A new generation of 99.999% enriched 28Si single crystals for the determination of Avogadro’s constant* Metrologia 54 (**2017**) 599

[5] O.C. Ernst, D. Uebel, S. Kayser, F. Lange, Th. Teubner, T. Boeck, *Revealing all states of dewetting of a thin gold layer on a silicon surface by nanosecond laser conditioning* Applied Surface Science Advances 3 (**2021**) 100040







Materials Science

Lab-based, quantitative X-ray diffraction imaging of strain and composition in bulk single crystals

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The variability of composition is one of the key parameters for tuning the physical properties of single-crystalline materials. Furthermore, during the growth of bulk single crystals, gradients of composition or doping are often observed. Any inhomogeneity within a single crystal will involve changes of the lattice parameters and, due to elastic interaction of these different regions, be a driving force for internal stresses or defect formation. A detailed knowledge about compositional variations and lattice strain is therefore important to optimize the crystal growth processes. Apart from that, substrate crystals with tailored lattice parameters serve as fundamental basis for the development of strained layers with outstanding physical properties [1]. For these reasons, the possibility to image the spatial variations of the crystal lattice is desirable for the growth and design of advanced single crystals.

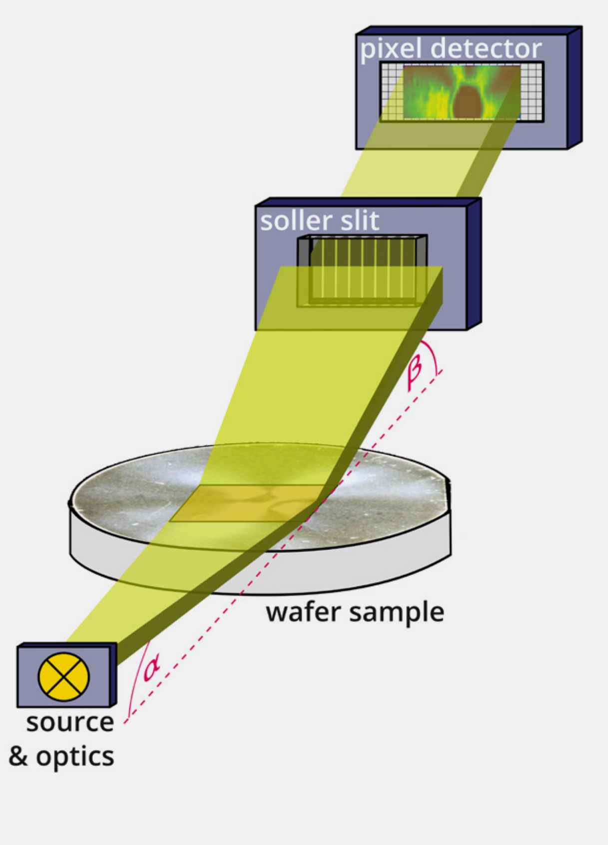

Fig. 1
XRD imaging geometry in the Rigaku SmartLab

In the field of semiconductor thin film technology, high-resolution X-ray diffraction (XRD) has become a routine tool to analyze the degree of strain and composition – particularly in the case of binary alloys. They key advantage of using XRD is the high sensitivity an easy access. To study inhomogeneities across wafers, it is common to perform XRD measurements at multiple spots on the surface. However, collecting the spatial distribution of XRD patterns is typically a technique used at synchrotron radiation sources [2, 3]. Benefiting from state-of-the-art lab-diffractometers and the availability of pixel detectors, it has become possible to perform high resolution XRD with spatial sensitivity corresponding to the pixel size in a manner similar to X-ray topography as illustrated in Fig. 1. The IKZ is operating a Rigaku SmartLab diffractometer capable of such imaging measurements. A one-to-one correspondence between detector pixel and sample position would be assured if the X-ray beam was parallel. However, since the beam is only collimated in the vertical regime (using a monochromator) the horizontal acceptance angle of the detector needs to be minimized by using so-called Soller slits. Provided by the minimum detector distance of 0.2 m and the best Soller slits available (0.114 °), the horizontal resolution is 0.4 mm, while the vertical resolution is limited by the detector pixel size, and therefore 0.1 mm at best. The field of view is limited to ~1mm x 6mm, but up to 4” wafers can be mapped by stitching several images after translating the sample horizontally.

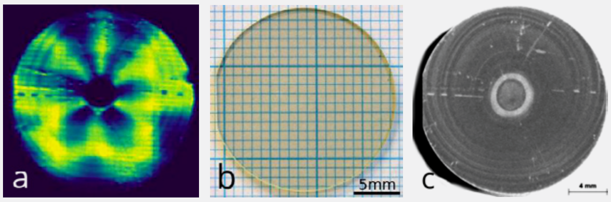

Fig. 2
XRD contrast image (a) compared to optical photograph (b) and energy dispersive Laue mapping (c) of a (0001) oriented wafer of (Mg,Zr):$SrGa_{12}O_{19}$

Fig. 2 shows a thus obtained XRD-contrast image next to an optical photograph for a 20 mm diameter, (0001) oriented wafer of a hexagonal (Mg, Zr): $SrGa_{12}O_{19}$ crystal – see the report in the Volume Crystals section on page 38/39 for details. Such images already give an impression about inhomogeneities in the crystal, since only regions light up that fulfill the Bragg condition for diffraction. To quantify the local deviation from the Bragg condition, the imaging procedure needs to be iterated for a series of incidence angles yielding a rocking curve I(α) for each spot on the surface. In general, there are two contributions that can locally change the Bragg condition and hence shift the rocking curve – a tilt of the diffracting net planes or a change of the interplanar spacing *d*. To disentangle these two contributions, the rocking curve imaging (RCI) is repeated after azimuthal rotation of 180 ° about the crystal surface normal, which inverts the effect of tilt but does not affect the shift due to changing interplanar spacing. By adding measurements at 90 ° azimuth, both lattice tilt components can be determined (see Fig. 3a). The tilt is a signature of stresses inside the crystal due to heterogeneous, elastically connected regions. In addition, the local rocking curves can be analyzed regarding their width, which is shown for a certain reflection in Fig. 3b and provides evidence for defects in the crystal as confirmed by a high-resolution Energy-dispersive Laue mapping (Fig. 2c).

The interplanar spacing *d* depends on all unit cell dimensions of the crystal. By determining the *d*-spacing for three non-coplanar Bragg reflections, we can determine the lattice parameters *a*, *b* and *c*. Based on these, the origin of heterogeneities in the crystal can be investigated. Typically, compositional changes result in a proportional scaling of the lattice parameters, whereas stresses result in a deformation and hence a change of the aspect ratio of the unit cell. By looking at the unit cell volume, we can isolate uniform scaling effects and hence study the spatial variation of chemical composition (Fig. 3c). Local changes of the unit-cell aspect ratio, as shown in Fig. 3d, highlight the distribution of local elastic strain.

For this crystal, it could be concluded that slight compositional changes connected to the crystallographic orientation of the phase boundary during growth are the driving force for lattice inhomogeneities and the entailed stress in the crystal. The co-doping with Mg^{2+} and Zr^{4+} (in partial substitution for Ga^{3+}) is more efficient on crystallographic planes with {1-10L} component compared to {11-2L} of the hexagonal lattice at the applied growth conditions and interface shape. Therefore, the expected 6-fold symmetry is observed in the map of the unit cell volume in Fig. 3c. Especially, a strong depression of unit cell size is found in the core part of the crystal where a (0001) facet formed during growth. The regions that connected strongly differing parts of the crystal, such as the ring surrounding the core and outer parts, are subjected to high stress, as can be seen in form of increased lattice tilt and a changing unit cell aspect ratio in Figs. 3a and 3d, respectively. The observed variation of unit cell size could be brought into good agreement with elemental analysis using X-ray fluorescence mappings and taking into account the ionic radii of Mg^{2+}, Zr^{4+} and Ga^{3+}. More details about complementary characterization, the material and the RCI technique can be found in a recently published paper [4].

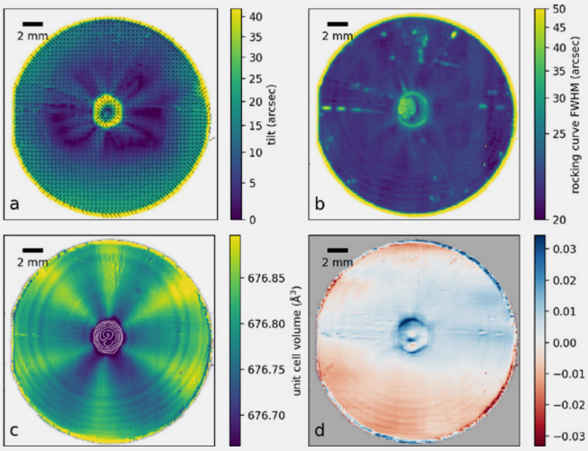

Fig. 3
RCI results. Lattice tilt (a), rocking curve width (b), unit-cell volume (c) and unit-cell aspect ratio (d) for the (0001) wafer of (Mg,Zr):$SrGa_{12}O_{19}$

References

[1] D. G. Schlom *et al.*, *MRS Bulletin*. **39**, 118–130 (2014).

[2] T. N. T. Caliste, A. Drouin, D. Caliste, C. Detlefs, J. Baruchel, *Applied Sciences*. **11**, 9054 (2021).

[3] A. Jafari *et al.*, *Journal of Applied Physics*. **121**, 044901 (2017).

[4] C. Guguschev, C. Richter *et al.*, *Cryst. Growth Des.* **22**, 4, 2557–2568 (2022).

Role of oxygen in the recovery of epitaxial AlN on sapphire

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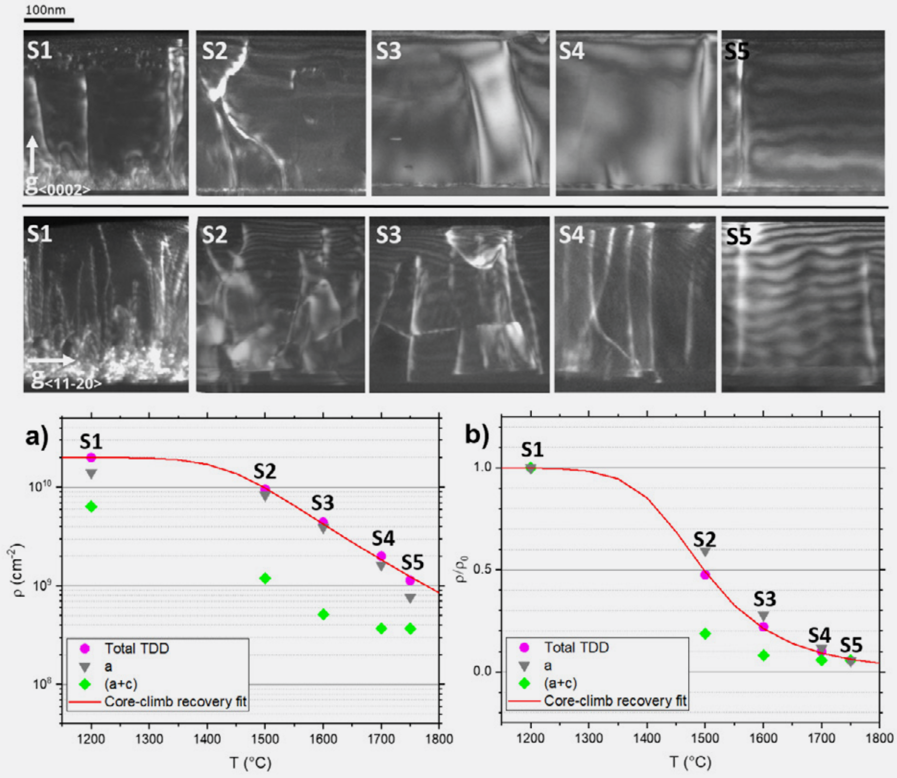

Fig. 1
TEM cross section micrographs of the AlN films as deposited (M1) and after isochronal annealing with increasing temperatures (1500°C M2, 1600°C M3, 1700°C M4, 1740°C M5). The mean density of threading dislocations reduces with increasing temperature.

Epitaxial AlN on sapphire is the most widespread pseudo-substrate for AlGaN-based UV light-emitting devices today. However, the large lattice mismatch between AlN and α-Al_2O_3 causes a high density of threading dislocations that negatively impact the performance of optoelectronic devices. Thermal annealing at 1500–1700 °C in a protective atmosphere (e.g., N_2) has been used efficiently to reduce the threading dislocations density (TDD) from the high 10^9 cm^{-2} range to the low 10^9 cm^{-2} range without the need to grow thick films or perform costly patterning processes. While devices fabricated on annealed templates show very promising improvement in the final device performance, this approach apparently has limitations, and a reduction in the dislocation density below 10^9 cm^{-2} seems challenging. Entangling the different processes that promote the reduction in threading dislocation density is therefore crucial and could help to optimize these pseudo-substrates further in a knowledge-based predictive approach. Fitting of experimentally measured data on threading dislocation densities from X-ray diffraction and TEM to phenomenological recovery models suggests that climb promoted by pipe diffusion of point defects along the dislocation core is the predominant mechanism. Such processes require high concentrations of intrinsic defects such as Al vacancies (V_{Al}), N vacancies (V_N), or vacancy complexes with impurities.

In the framework of collaborative work between the IKZ and groups at Ferdinand-Braun-Institut and North-Carolina State University we study the role of oxygen in the recovery process of AlN films during high temperature annealing by SIMS and transmission electron microscopy-based methods. [2] Oxygen is a natural impurity in Al containing compounds and is present at abundant amount in the sapphire substrate. In the AlN films it acts as a donor and reduces the formation of V_{Al} and V_N and complexes of these vacancies with O, promoting recovery by dislocation climb. Fig. 1 shows cross sectional transmission electron micrographs of an AlN layer after isochronal annealing at temperatures between 1500°

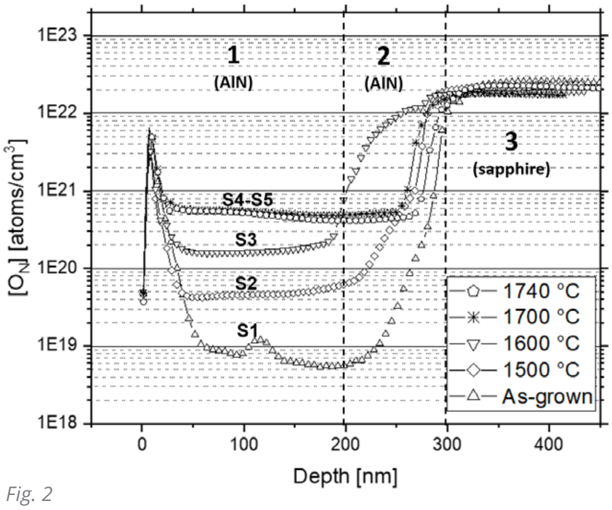

Fig. 2

Oxygen profiles of as grown and annealed AlN samples obtained by secondary ion mass spectrometry. An oxygen plateau is visible for all samples. Its value depends on the annealing temperature.

and 1740°C. The threading dislocation density decreases rapidly with increasing annealing temperature and saturates at a value of $1x10^9$ cm^{-2}. Further reduction is not possible even at significant longer annealing times.

Fig. 2 shows the oxygen concentration profiles of the layers as measured by secondary ion mass spectroscopy. The oxygen profiles exhibit a plateau-like behavior increasing from 5-8 × 10^{18} cm^{-3} in the as-grown sample to 5-8 × 10^{20} cm^{-3} for the sample annealed at 1700 °C. Though these plateaus suggest to be related to the solubility limit of oxygen in AlN at the given temperature, this would require diffusion of oxygen through the whole layer, which is inconsistent with experimentally measured diffusion coefficients for oxygen in bulk AlN for the given annealing time and temperature.

To explain the saturation of the oxygen concentration we therefore consider a mixed pipe/bulk diffusion model that describes oxygen diffusion by bulk diffusion from the substrate into the layer by fast pipe diffusion through the dislocation core and radial bulk out-diffusion from threading dislocations into the bulk as shown schematically in Fig. 3. Within the considered cylindrical volume, given by the bulk diffusion length of oxygen and the dislocation length, the oxygen reaches its thermodynamical saturation limit. It is the high oxygen concentration that in turn promotes the formation of $(V_{Al}–2O_{N})$ complexes and O_N. From the comparatively low formation enthalpy (0.75 eV), very high concentrations of vacancies are expected to form, promoting dislocation climb and thereby mutual annihilation of dislocations with same Burgers vector but opposite line direction. The experimentally found limit for the reduction in dislocation densities by thermal annealing can therefore be explained by the transition from an oxygen diffusion that follows predominantly the mixed diffusion along the dislocations into the bulk to an effective bulk diffusion. With decreasing threading dislocation density during the annealing, the effective diffusivity decreases, while the average dislocation distance increases. Below a certain dislocation density bulk diffusion is predominant, which slows the climb process down. An estimate shows that this transition occurs at a dislocation density around 10^9 cm^{-2} corresponding to the lowest threading dislocation density in these layers.

An alternative way to promote injection of vacancies in AlN layers s through emission from nanopipes, hollow tubes with a diameter of few nanometer aligned along the surface normal of the film. Such nanopipes form during growth if high concentrations of oxygen are present at the growth surface. We could show [2] hat they transform into faceted voids acting as an efficient vacancy source during annealing of the film. The transformation of nanopipes to voids and the shrinkage of these voids upon annealing is described in terms of classical sintering theory. Intentionally creating nanopipes (e.g. changing parameters during growth, or by electrochemical etching) in AlN layers before annealing could thus be an efficient way to further reduce the threading dislocation density in AlN layers.

References

[1] L. Cancellara, T. Markurt, T. Schulz, M. Albrecht S. Hagedorn, S. Walde, S. Washiyama, M. Weyers, R. Collazo, Z. Sitar, and M. Albrecht, J. Appl. Phys. 130, 203101 (2021); doi: 10.1063/5.0065935

[2] L. Cancellara, S. Hagedorn, S. Walde, D. Jaeger, and M. Albrecht, J. Appl. Phys. 131, 215304 (2022); doi:10.1063/5.0088948

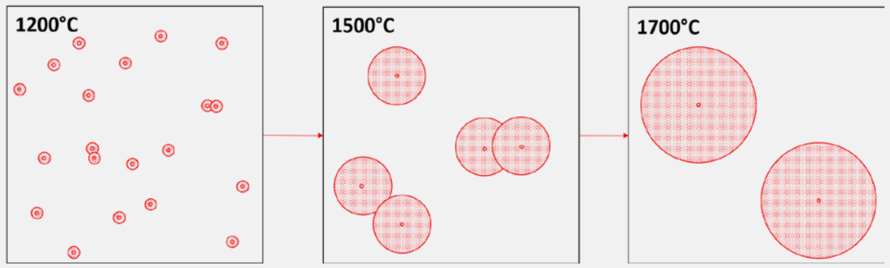

Fig. 3

Schematic top view of the diffusion cylinders. As the annealing temperature is increased, the cylinders' density decreases due to the annihilation of dislocations.At the same time the radius increases since it is determined by oxygen bulk diffusivity. The balance between these two parameters determines the oxygen-saturated volume fraction.

Towards understanding and optimization of VGF-GaAs crystal growth process

using data mining and machine learning techniques

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Development and optimization of bulk crystal growth processes is a difficult task due to the multidisciplinarity of the phenomena associated with the melt-crystal phase change, numerous technological parameters, and in particular, the dynamic nature of the process with a considerable time delay between a change of a growth parameter and the system response, e.g. at the crystal-melt interface.

In our study reported in [1], the task of process understanding and optimization was approached by combining several data mining (DM) techniques with machine learning (ML) methods: with the latter we mean the decision trees (DT), i.e. regression (RT) and classification (CT) trees. These methods were chosen, while bulk crystal growth is viewed as a field, where only small data amounts are available, and where training data is expensive to produce or difficult to obtain from proprietary sources. In the end the goal was to derive, optimize and understand the factors influencing the vertical gradient freeze (VGF) crystal growth process.

As a process example, VGF-GaAs growth of 4-inch crystals was used, due to the strong interest in III-V crystals as materials for the next generation of wireless communications. All selected data techniques were used to understand, quantify and rank influences of growth rate and the power of heaters on the interface deflection and maximal temperature in GaAs in order to grow low-cost high-quality crystals. The latter is characterized among others by a high growth velocity and by a flat solid/liquid interface. Training data were generated by 2-dimensional computational fluid dynamics (CFD) simulations (Figure 1). The furnace geometry corresponded to a commercial furnace with five graphite resistance heaters. The CFD simulations were performed using commercial code CrysMAS.

For the generation of training datasets for ML simulations, 130 combinations of heating power in 5 heaters in the range from 0–4 kW and growth rates in the range 0.1–5.4 mm/h were used as input parameters for the CFD simulations. The interface deflection was measured at the melt symmetry axis. The DM techniques were used in this study before ML with the aim of assessing the quality of the training data and examining their relationships. As ML techniques we applied regression trees (RT) and classification trees (CT) for the accurate prediction of VGF-GaAs growth recipes and easy understanding of the role of various process parameters. Concerning RT the target variables are real numbers. The target variables of CTs are labels of classes. As the name says, all DT algorithms have a tree structure (Fig. 2): each node in the tree represents a variable from the input datasets, each branch a decision and each leaf at the end of a branch the corresponding output value.

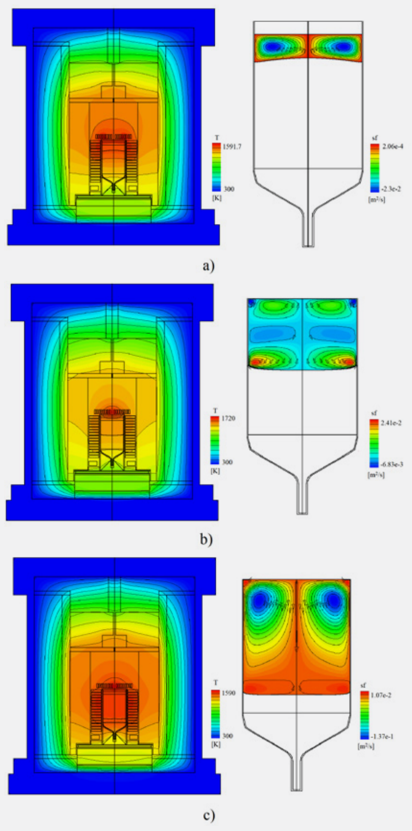


Fig. 1

Examples of CFD results for the temperature in the furnace and the stream function in GaAs melt for various growth recipes and percentage of crystalized GaAs.

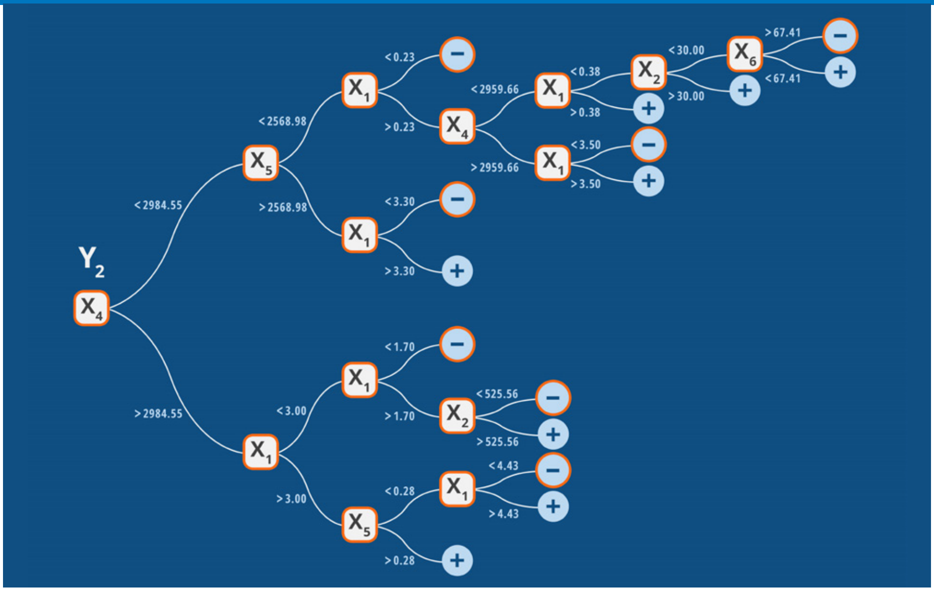


Fig. 2
Classification tree analyzing the dependence of the solid-liquid interface deflection y2 on the power of heaters, i.e. inputs x1-x6. Red frames correspond to branches where leaf nodes have mean deflection y2<0, i.e. convex shape of s/l interface.

The training data were identical to those used in DM analysis and consisted of the 130 data sets. For assessing the effect of various inputs on specific output, regression and classification tree analysis and the comparison of mean output values were applied. For both kinds of DT simulations, the commercial software Matlab® was used.

Correlation analysis was used to study the degree to which the variables, both inputs and outputs, are associated with each other. The most pronounced correlation among inputs was observed for the power of the two side heaters. Concerning outputs, e.g. interface deflection, it is the most negative correlated by the increase of the power of upper side heater and the most positive correlated by the increase of the power of top inner heater. For the GaAs temperature at the melt free surface, the most pronounced negative correlation (weak with beneficial influence) have inputs: the power of upper side heater and growth rate, since they decrease this temperature value and therewith they limit severe arsenic evaporation.

A successful VGF process is characterized among others by a flat crystallization front during the growth and constrained maximal temperatures in the melt to prevent strong arsenic evaporation/loss. The purpose of the DT analysis was to better understand the role of various process parameters and to identify their suitable values for the growth of high-quality crystals.

The resulting RT for interface deflection reveals the heating power of the inner top heater followed by upper side heater and growth rate, as the most decisive inputs for the favorable flat or slightly convex interface shape. Their significance decreases in the order mentioned above.

The same optimization task for interface deflection was also solved using a classification tree.

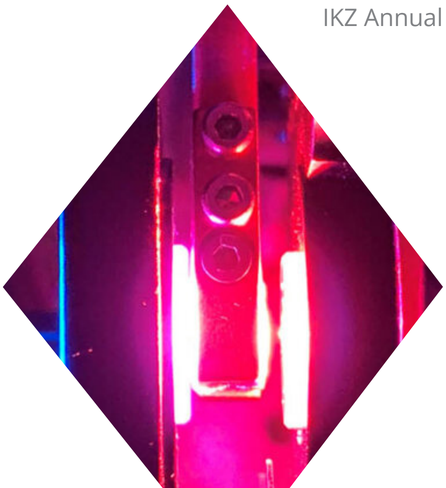
As with the RT, the CT results showed that during the rapid growth of crystals with a slightly convex interface, the process heat should mainly be provided by the upper side heater (Figure 2). The resulting RT for predicting the most influential input to keep the GaAs temperature below the limits for high arsenic evaporation pointed out the heating power in the bottom heater, followed by the heating power in the upper side heater.

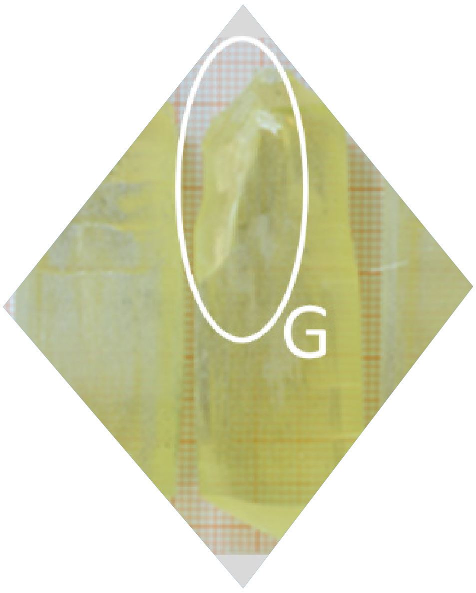
This study demonstrated the capabilities of data mining and machine learning in smart derivation of the crystal growth recipes on the example of VGF-GaAs growth. The decision trees, both regression and classification type, are an excellent choice if we need a machine learning model with short training times based on a low volume of CFD training data able to provide human-comprehensible results. The decision trees also provide ranges of process parameters (e.g., power of heaters and growth rate) where nearly-optimal values of the output variables (e.g., interface deflection or maximal temperature in GaAs) can be found.

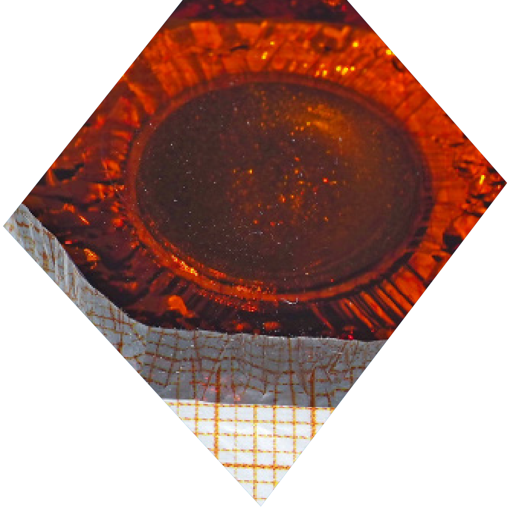
The proposed combination of two modern data-driven techniques and standard CFD modeling can be easily further deployed in the fast development of the novel crystal growth processes/grown materials, as well as their scale up.

Reference

[1] N. Dropka, K. Böttcher, M. Holena, Development and optimization of VGF-GaAs crystal growth process using data mining and machine learning techniques, Crystals 11 (2021) 1218.







Application Science

Miniaturized short-pulse laser in the visible spectral range

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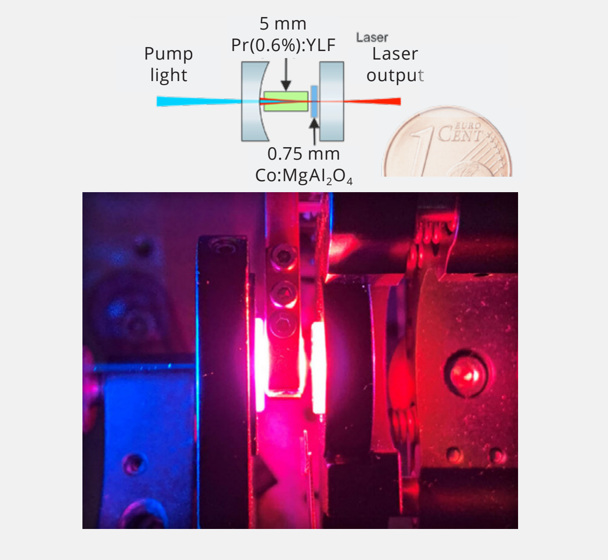


Fig. 1
Picture and sketch of the pulsed Pr:YLF laser.
The 1-cent coin serves as a true-to-scale size comparison.

The Nobel-prize winning invention of blue-emitting InGaN-based laser diodes led to a revival of rare earth-doped solid-state lasers with direct emission in the visible spectral range. In fact, most of the optically active trivalent rare earth ions exhibit absorption lines in the blue spectral range, which enable pumping with these emerging laser diodes. In particular, trivalent praseodymium (Pr^{3+}) attracted many researchers because of its various strong visible emission lines. This resulted in the development of highly efficient diode-pumped visible solid-state lasers based on Pr^{3+}, some of which are meanwhile commercially available.

Pulsed laser operation is beneficial for many applications. By compressing the energy into a brief period of time in laser pulses, the instantaneous laser power is enhanced by several orders of magnitude. This is advantageous for many applications, *e.g.*, in micromachining of metals or semiconductors, where pulsed lasers deposit less heat in surrounding areas and thus enable highly precise material processing. For the same reason, pulsed lasers are used in soft-tissue surgery, in order to prevent necrosis by overheating the surrounding tissue. The high peak power levels of pulsed lasers are also useful to drive nonlinear frequency conversion processes, as the conversion efficiency increases with laser peak power. Furthermore, in science, short laser pulses are required as "flash lights" for the time-resolved investigation of fast processes.

Commonly, host materials doped with trivalent neodymium (Nd^{3+}) or erbium (Er^{3+}) are used for Q-switching, where laser pulses are formed by a periodic modulation of the losses inside the cavity. These systems have been extensively studied in the past and meanwhile allow to achieve sub-ns pulse durations and pulse energies of several joules. However, Nd^{3+}- and Er^{3+}-based lasers emit light in the infrared spectral range, but the prospects of Q-switching in the visible using Pr^{3+} as the active ion have not yet been studied in detail.

Corresponding investigations have now been conducted at IKZ’s Center for Laser Materials by adopting the well-known tetragonal host material lithium yttrium fluoride (YLF) for Pr^{3+}. The short laser pulses were realized by passive Q-switching, *i.e.*, by placing a saturable absorber, in which the transmission increases at high light intensities, into the laser cavity. In this way, pulsed laser operation is favoured over continuous-wave emission. Unlike active Q-switching, no expensive and complex electronics or bulky mechanics are required in a passively Q-switched laser setup. A well-established approach to achieve the shortest pulse durations from passively Q-switched lasers is minimizing the cavity length. To this end, a cavity configuration with a length well below 1 cm was set up (see Fig. 1). Such a compact solution imposes additional challenges: obtaining a high efficiency of the laser is more difficult because of fewer degrees of freedom in the alignment of the optical components compared to longer cavities, which also makes it difficult to compensate for destabilizing thermal lensing effects at high pump powers. By the systematic investigation of different cavity configurations and properties of the divalent cobalt (Co^{2+})- doped spinel saturable absorber crystal, Q-switched pulses shorter than 10 ns were achieved at wavelengths of 640 nm in the red and 607 nm in the orange spectral range, for the first time.

Co^{2+}-doped saturable absorbers are usually applied for Q-switching of lasers with emission in the telecom-band around 1.5 µm. The recent work shows that this widely commercially available saturable absorber material is also highly suited for the generation of short Q-switched pulses in the visible spectral range. A critical factor for achieving stable laser pulses at shortest durations is the modulation depth of the saturable absorber, which is defined as the change in transmission between low and high incident light intensity. At 4 W of 480-nm blue pump power, a comparably low modulation depth around 3% yielded pulse repetition rates of up to 1 MHz at a wavelength of 640 nm in our setup. In this case, the average laser output power amounted to more than 1 W.

In contrast, a higher modulation depth of 20% increased the cavity losses and thus decreased the efficiency of the laser, resulting in only 0.29 W of average output power, however, at lower pulse repetition rates around 100 kHz. For the orange laser an even lower repetition rate of 48 kHz at 0.34 W of average output power was achieved. In the strong-modulation-depth regime around 20%, the pulse durations are reduced to 2.3 ns and 5.3 ns at 640 nm and 607 nm, respectively. These are more than a factor of three below the durations for lower modulation depth and represent the shortest ever recorded pulse durations of any Q-switched Pr^{3+}-based laser to date.

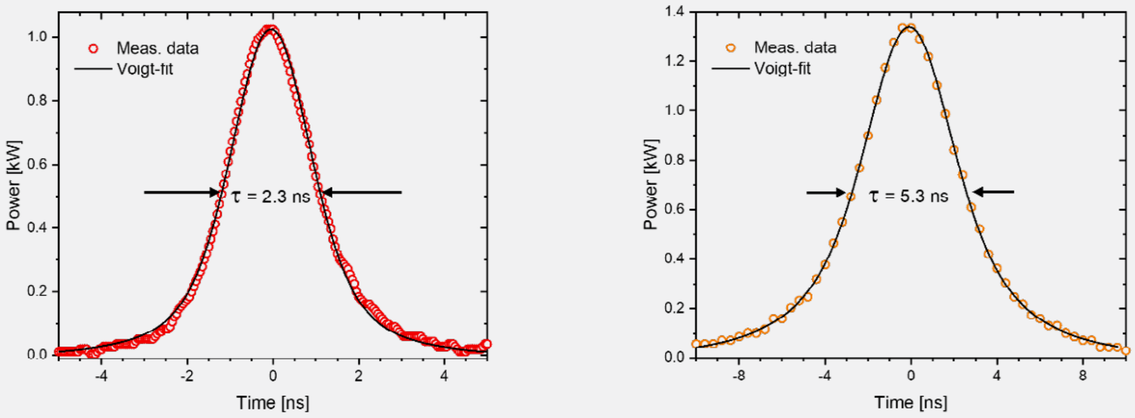
The reduction in pulse repetition rate and pulse duration in the strong-modulation-depth regime led to a significant enhancement of the pulse peak power to more than 1 kW in the red at 640 nm and even 1.3 kW in the orange at 607 nm. Due to the significantly lower gain for the green transition of Pr^{3+} at 523 nm, this laser could not be operated with high modulation depths and consequently, pulse durations below 100 ns were not achieved.

This laser provides a simple and compact approach for the generation of short pulses with kW-class peak power levels in the visible with the opportunity for further peak power scaling. It is suitable for the application as a narrow bandwidth, short-pulsed seed laser in a seed-amplifier system for high average power visible laser emission and exhibits a great flexibility in terms of operation parameters such as repetition rate, pulse energy and average power enabled by adjusting the saturable absorber thickness and/or doping concentration. Additionally, the achieved high peak powers are beneficial for the efficient generation of coherent ultraviolet (UV) radiation in a compact and cost-effective device by a single step of nonlinear frequency conversion of the visible laser output. More details on this laser can be found our recent publication published in the journal of Applied Physics B [1].

Reference

[1] Badtke, M. et al. „Passively *Q*-switched 8.5-ns Pr^{3+}:YLF laser at 640 nm". *Appl. Phys. B* **127,** 83 (2021). https://doi.org/10.1007/s00340-021-07629-2

Fig. 2
Temporal power profiles and Voigt-fits of the shortest pulse of any Q-switched praseodymium laser to date recorded at 640 nm (left) and of the highest peak power pulse obtained in the orange at 607 nm (right)



AlN – diameter increase – 10 mm prototype substrates and progress towards 1 inch

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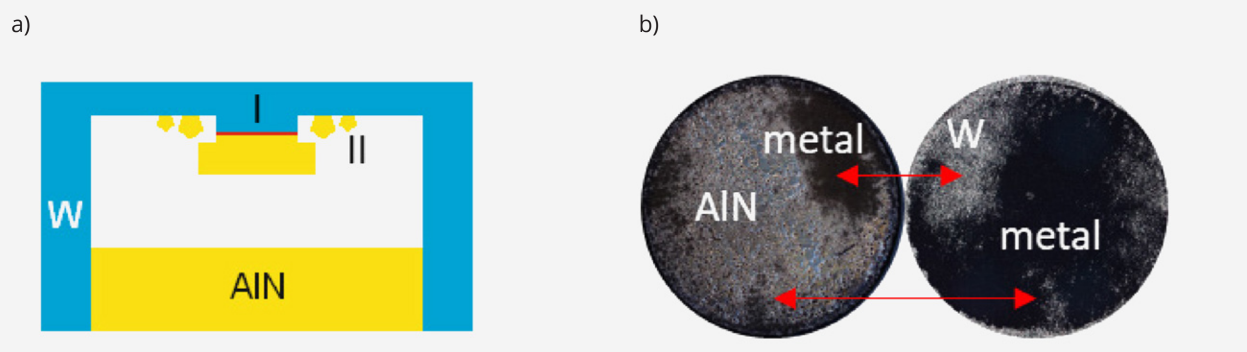
AlN is a promising substrate material for AlGaN-based UVC light emitting devices [1] in particular for short wavelength (< 270 nm) and corresponding high Al content but also for other applications in power- and high-frequency electronics or high temperature sensors. AlN substrates are commercially available only in limited number and with few pre-defined specifications. For this reason, IKZ develops AlN substrates with diameters between 10 and 25 mm as prototype series with flexible specifications for research on new electronic components.

Major challenges in growing AlN crystals by the sublimation method are the suspending mounting of the single-crystalline seed at the top of the crucible and the separation of polycrystalline AlN growing next to the seed, which normally hinders an increase of the crystal diameter and leads to stresses and defect formation at the crystal rim when in contact with the growing crystal. IKZ recently developed a process with seed fixation on an elevated seed holder prior to the actual growth process enabling growth of the crystal without contact to the polycrystalline grains (Fig. 1a) and significant diameter increase by lateral growth. The seed attachment was realized by bonding a metallic intermediate layer with the seed back and the seed holder top at temperatures above 1000°C and a contact pressure of approx. 1 bar (Fig. 1b).

Fig. 1
a) Schematic drawing of a crystal growth setup with elevated seed (I) and polycrystalline growth (II).
b) Interface between seed backside and seed pedestal after intentional separation after seed fixation showing a broken metallic interlayer with residuals on both surfaces.



The growth evolution of an AlN crystal grown on a 5 mm seed without contact to polycrystalline grains and strong lateral expansion is shown in the transmission image of an axial cut parallel to the a-plane in Fig. 2a. Areas with different color can be attributed to different growth modes. The dark layer with approx. 300 µm thickness on top of the seed surface is caused by high oxygen concentration which is not unusual for the initial growth and strong oxygen release from the source material. The color of the main volume is typical for c-plane spiral growth on N-terminated surfaces while the bright areas at the crystal rims indicate m- and r-plane growth. A monochromatic beam X-ray topography (MB-XRT) image taken with weak beam contrast at +0.002° deviation from the rocking curve peak of the 1-100 reflection (Fig. 2b) with its considerably enhanced dislocation contrast and spatial resolution reveals that the dislocation density in the bulk volume above the seed is similar to the density in the seed (Fig. 2c) and that the volume on the left side next to the seed is dislocation-free.

With the help of 3D-reconstruction the typical course of dislocations at the interface between seed and bulk volume could be identified as shown in Fig. 2d. After leaving a horizontal dislocation network on the seed surface in vertical direction (Fig. 2d-2) the dislocations run horizontally in the area with high contrast and then turn vertically with slight inclination to the c-axis in the main bulk volume. As the dislocation trajectories are located in a-planes and not in m-planes as we would expect for glide-processes they are probably formed by impurity enhanced climb-processes during growth.

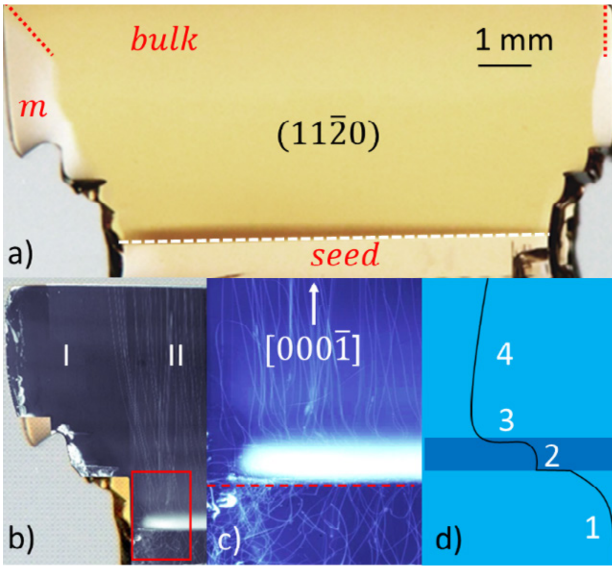


Fig. 2:
Axial a-plane cut through AlN crystal grown on seed.

a) Transmission picture with seed and several bulk-grown areas with different color correlated to local growth conditions.

b) MB-XRT picture of left side using the 1-100 reflection with an area of a-type dislocations aligned along the c-direction (II) and an area free of dislocations (I).

c) Magnified MB-XRT picture of interface between seed and bulk volume with different dislocation arrangement in seed and bulk volume.

d) Typical dislocation course at interface between seed and bulk volume.

In 2018 process development and diameter increase (Fig. 3) was started from 5 mm spontaneous nucleated seeds with excellent crystalline quality and dislocation densities in the range 10^3 cm^{-2} to 10^4 cm^{-2}. Meanwhile crystals with 10 mm diameter can be reproducibly grown and we are able to manufacture prototype substrate series for research with tailor made specifications for different applications. Presently the focus is on AlGaN-based light emitting diodes and laser diodes which require a damage free chemical mechanical polished surface and a tight off-orientation specification around 0.20° which can be efficiently measured with a new commercial equipment acquired in 2021 using the omega-scan technology developed by the German manufacturer Freiberg Instruments GmbH. In the future, the suitability of the substrates will also be evaluated for other applications and specifications will be adapted if necessary.

Parallel to the evaluation and optimisation of the substrates with 10 mm diameter, the diameter expansion is to be driven forward based on the existing process technology. Meanwhile a process for substrate diameters up to 25 mm could be demonstrated and the availability of 1" prototype substrates is planned for 2025.

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References

[1] M. Kneissl, T.Y. Seong, J. Han and H. Amano,
The emergence and prospects of deep-ultraviolet light-emitting diode technologies,
Nature Photonics 13, 233 (2019).

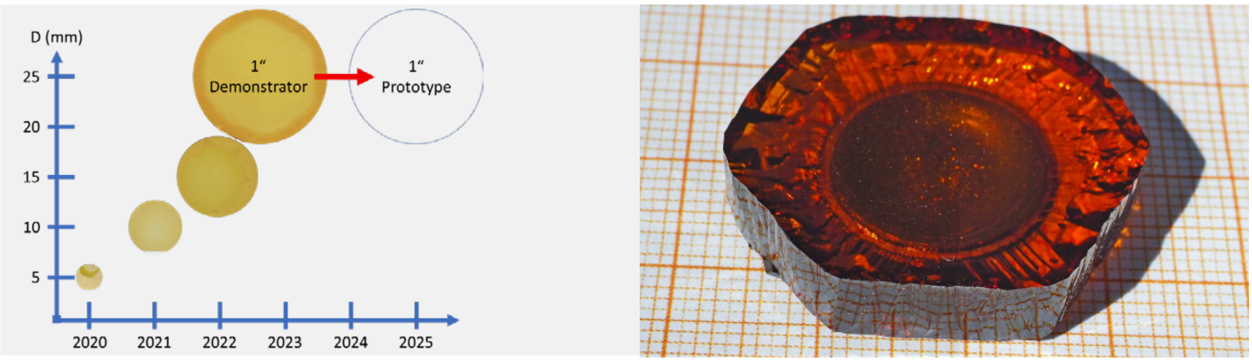

Fig. 3
Left - Illustration of diameter increase for AlN substrates at IKZ showing transmission light images of a 5 mm seed prepared from spontaneous nucleated crystals (2020) as well as substrates grown on seeds with 10 mm (prototype), 15 mm and 25 mm diameter (demonstrator).
Right – 1-inch demonstrator crystal.

Gallium oxide substrates for future power electronics – prototype technology challenges

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Mainly due to its high theoretical breakdown field (8 MV/cm) gallium oxide is one of the most promising materials for the next generation of power electronic devices. Presently a multitude of test power devices with lateral and vertical device structure are under development worldwide [1] utilizing gallium oxide substrates with different specifications, in particular different orientations (e. g. 100, 010, 001), various offcuts and doping (e. g. semi-insulating, n-doped). IKZ has pioneered bulk growth of gallium oxide single crystals by the Czochralski (CZ) method and has since demonstrated 2-inch diameter crystals with unprecedented volume and structural quality.

In 2021 IKZ started the BMWi-funded project "GO-Wafer" together with the industry partner CrysTec GmbH on the commercialization of gallium oxide (Ga_2O_3) substrates for this research market, e.g. the development of power electronic devices. During the project, the entire substrate manufacturing line is to be tested with regard to its technological capability and, if necessary, technologies are to be optimised. It will also be evaluated whether the technologies are suitable for efficiently producing substrates with variable specifications, in particular with different doping levels and orientations. Special focus will be put on the material-efficient sawing of the crystals with controlled off-orientation, which is a particular challenge for the material Ga_2O_3 with its strong tendency to cleave along the planes (100) and (001).

Crystals with variable bulk specifications will be grown at IKZ with the CZ method and then be used at CrysTec for the development of efficient sawing and polishing processes adapted to the respective volume properties and orientation. Additionally, substrates will be evaluated by epitaxy at IKZ ([2, 3], see also report in the Nanostructures & Layers section) and if needed epitaxy or wafering processes will be optimized for an optimal overall performance.

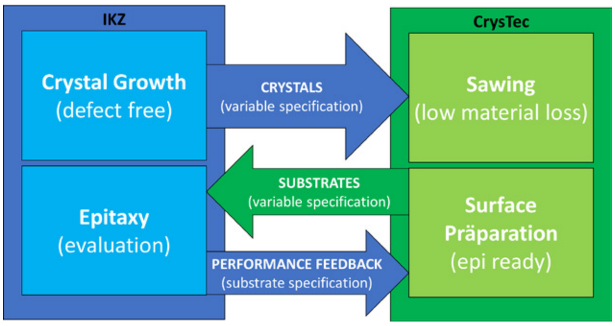

Fig. 1
Schematic illustration of GO-Wafer project structure including work packages Growth (AP1), Sawing (AP3), Polishing (AP3) and Epitaxy (AP4) as well as material and information flow.

Ga_2O_3 crystals are successfully grown by the Czochralski method at IKZ since several years by Galazka et al. [4, 5] and crystals with different doping and excellent quality were demonstrated but still a significant share cannot be used for substrate preparation mainly due to grain and twin defects as illustrated in Fig. 2.

The presence of these crystalline defects is not relevant for small substrates for basic research as these can be prepared from the defect free crystal volume by cleavage but must be avoided for the efficient preparation by sawing with variable orientation in particular for larger substrate sizes.

As the existing process has already demonstrated its capability to produce defect free crystals, the focus of the project will be to reduce the variation of process parameters from process to process and then narrow down the existing process window for maximum yield.

In particular the following strategies will be applied to achieve this goal:

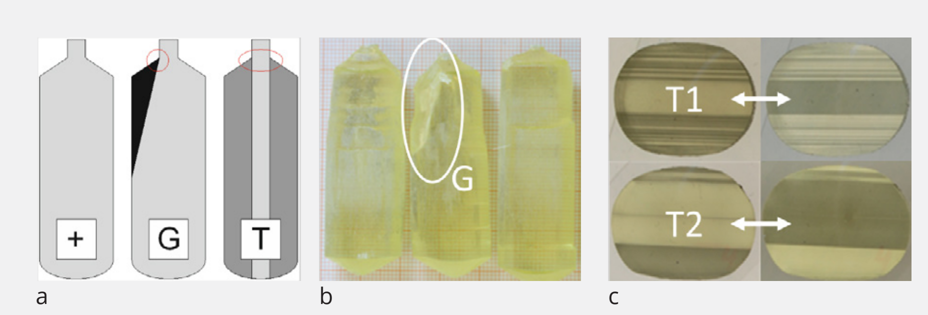

Fig. 2

a) Schematic illustration of a perfect crystal (+), grain (G) and twin (T) defects in Ga_2O_3 crystals.

b) Typical Ga_2O_3 crystals and grain defect generated at the seed rim.

c) Transmission images of two crystals (T1, T2) taken with crossed polarizers along the b-direction with typical twin defect patterns.

I. Improvement of the equipment – e.g. by improving seed-holder technology
II. Implementation of additional measurement tools – e.g. a temperature measurement on the crucible bottom and rim
III. Process data should be electronically pre-processed and made accessible for evaluation with artificial intelligence tools.

To prevent Ga_2O_3 substrates from splitting during the sawing process along the light cleavage planes (100) and (001), embedding in a suitable polymer matrix is mandatory. In particular, it must be ensured that no stresses occur during cooling or curing that could lead to cracking of the polymer matrix and the embedded Ga_2O_3 disc after sawing.

Basic tests with different sawing parameters have also shown that a stable wire guiding and low vertical advance as well as a positioning of the crystal with vertical alignment of the (001) direction is favourable.

With optimized embedding and sawing parameters crack free sawing of 20 mm crystals perpendicular to the (010) growth direction was successfully demonstrated.

This process will now be also tested and modified if required for the sawing of (100) substrates with 4° off-orientation.

Acknowledgements

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References

[1] https://www.adlershof.de/news/galliumoxid-leistungstransistoren-mit-rekordwerten/

[2] S. Bin Anooz et al., Step flow growth of β-Ga_2O_3 thin films on vicinal (100) β-Ga_2O_3 substrates grown by MOVPE, Appl., Phys. Lett., Vol. 116, 182106, 2020.

[3] S. Bin Anooz et al., Impact of chamber pressure and Si-doping on the surface morphology and electrical properties of homoepitaxial (100) β-Ga_2O_3 thin films grown by MOVPE, J. Phys. D: Appl. Phys., Vol. 55, 034003, 2021.

[4] Z. Galazka et al., β-Ga_2O_3 for wide-bandgap electronics and optoelectronics, Semicond. Sci. Technol., Vol. 33, 113001, 2018.

[5] Z. Galazka et al., Bulk single crystals of β-Ga_2O_3 and Ga-based spinels as ultra-wide bandgap transparent semiconducting oxides, Progress in Crystal growth and Characterization of Materials, Vol. 67, 100511, 2021.

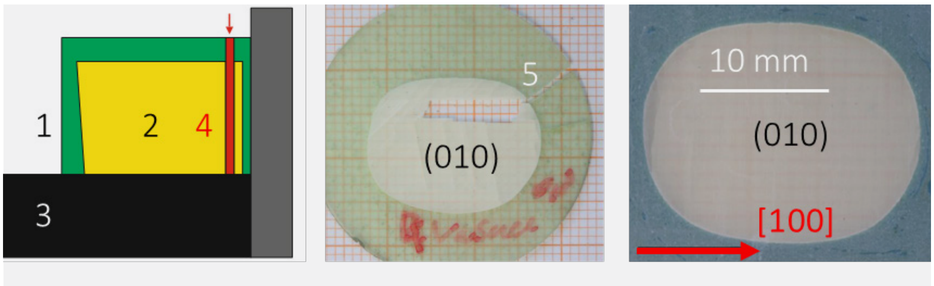

Fig. 3

a) Schematic illustration of sawing process of embedded (1) Ga_2O_3 crystal (2) on graphite holder (3) with wire sawing (4) parallel to the 010 plane.

b) Sawed Ga_2O_3 wafer with crack through embedding material (5) and Ga_2O_3 substrate.

c) Sawed substrate with improved embedding sawed along the [100] direction without cracking.

Appendix

Publications

Publications in peer-reviewed journals

Abdullayev, A., Klimm, D., Kamutzki, F., Gurlo, A., Bekheet, M.F., *AlF_3-assisted flux growth of mullite whiskers and their application in fabrication of porous mullite-alumina monoliths.* Open Ceramics 7 (2021), 100145.

Agostini, M.; Araujo, G.; Bakalyarov, A. M.; Balata, M.; Barabanov, I.; Baudis, L.; Bauer, C.; Bellotti, E.; Belogurov, S.; Bettini, A.; Bezrukov, L.; Biancacci, V.; Bossio, E.; Bothe, V.; Brudanin, V.; Brugnera, R.; Caldwell, A.; Cattadori, C.; Chernogorov, A.; Comellato, T.; D'Andrea, V.; Demidova, V.; DiMarco, N.; Doroshkevich, E.; Fischer, F.; Fomina, M.; Gangapshev, A.; Garfagnini, A.; Gooch, C.; Grabmayr, P.; Gurentsov, V.; Gusev, K.; Hakenmuller, J.; Hemmer, S.; Hofmann, W.; Huang, J.; Hult, M.; Inzhechik, L. V.; Janicskó Csathy, J.; Jochum, J.; Junker, M.; Kazalov, V.; Kermaidic, Y.; Khushbakht, H.; Kihm, T.; Kirpichnikov, I. V.; Klimenko, A.; Kneissl, R.; Knopfle, K. T.; Kochetov, O.; Kornoukhov, V. N.; Krause, P.; Kuzminov, V.; Laubenstein, M.; Lindner, M.; Lippi, I.; Lubashevskiy, A.; Lubsandorzhiev, B.; Lutter, G.; Macolino, C.; Majorovits, B.; Maneschg, W.; Manzanillas, L.; Miloradovic, M.; Mingazheva, R.; Misiaszek, M.; Moseev, P.; Muller, Y.; Nemchenok, I.; Pandola, L.; Pelczar, K.; Pertoldi, L.; Piseri, P.; Pullia, A.; Ransom, C.; Rauscher, L.; Riboldi, S.; Rumyantseva, N.; Sada, C.; Salamida, F.; Schonert, S.; Schreiner, J.; Schutt, M.; Schutz, A. K.; Schulz, O.; Schwarz, M.; Schwingenheuer, B.; Selivanenko, O.; Shevchik, E.; Shirchenko, M.; Shtembari, L.; Simgen, H.; Smolnikov, A.; Stukov, D.; Vasenko, A. A.; Veresnikova, A.; Vignoli, C.; von Sturm, K.; Wester, T.; Wiesinger, C.; Wojcik, M.; Yanovich, E.; Zatschler, B.; Zhitnikov, I.; Zhukov, V.; Zinatulina, D.; Zschocke, A.; Zsigmond, A. J.; Zuber, K.; Zuzel, G. (GERDA Collaboration), Characterization of inverted coaxial 76Ge detectors in GERDA for future double-β decay experiments. Eur. Phys. J. C **8** (2021) 505.

Aggoune, W.; Irmscher, K.; Nabok, D.; Vona, C.; Bin Anooz, S.; Galazka, Z.; Albrecht, M.; Draxl, C., *Fingerprints of optical absorption in the perovskite $LaInO_3$: Insight from many-body theory and experiment.* Physical Review B; **103** (2021), 115105.

Agostini, M.; Araujo, G.; Bakalyarov, A. M.; Balata, M.; Barabanov, I.; Baudis, L.; Bauer, C.; Bellotti, E.; Belogurov, S.; Bettini, A.; Bezrukov, L.; Biancacci, V.; Bossio, E.; Bothe, V.; Brudanin, V.; Brugnera, R.; Caldwell, A.; Cattadori, C.; Chernogorov, A.; Comellato, T.; D'Andrea, V.; Demidova, V.; DiMarco, N.; Doroshkevich, E.; Fischer, F.; Fomina, M.; Gangapshev, A.; Garfagnini, A.; Gooch, C.; Grabmayr, P.; Gurentsov, V.; Gusev, K.; Hakenmuller, J.; Hemmer, S.; Hiller, R.; Hofmann, W.; Huang, J.; Hult, M.; Inzhechik, L. V.; Csathy, J. J.; Jochum, J.; Junker, M.; Kazalov, V.; Kermaidic, Y.; Khushbakht, H.; Kihm, T.; Kirpichnikov, I. V.; Klimenko, A.; Kneissl, R.; Knopfle, K. T.; Kochetov, O.; Kornoukhov, V. N.; Krause, P.; Kuzminov, V.; Laubenstein, M.; Lindner, M.; Lippi, I.; Lubashevskiy, A.; Lubsandorzhiev, B.; Lutter, G.; Macolino, C.; Majorovits, B.; Maneschg, W.; Manzanillas, L.; Miloradovic, M.; Mingazheva, R.; Misiaszek, M.; Moseev, P.; Muller, Y.; Nemchenok, I.; Pandola, L.; Pelczar, K.; Pertoldi, L.; Piseri, P.; Pullia, A.; Ransom, C.; Rauscher, L.; Riboldi, S.; Rumyantseva, N.; Sada, C.; Salamida, F.; Schonert, S.; Schreiner, J.; Schutt, M.; Schutz, A. K.; Schulz, O.; Schwarz, M.; Schwingenheuer, B.; Selivanenko, O.; Shevchik, E.; Shirchenko, M.; Shtembari, L.; Simgen, H.; Smolnikov, A.; Stukov, D.; Vasenko, A. A.; Veresnikova, A.; Vignoli, C.; von Sturm, K.; Wester, T.; Wiesinger, C.; Wojcik, M.; Yanovich, E.; Zatschler, B.; Zhitnikov, I.; Zhukov, V.; Zinatulina, D.; Zschocke, A.; Zsigmond, A. J.; Zuber, K.; Zuzel, G. (GERDA Collaboration), *Calibration of the GERDA experiment.* European Physical Journal C; **81** (2021), 682.

Agostini, M.; Araujo, G.; Bakalyarov, A. M.; Balata, M.; Barabanov, I.; Baudis, L.; Bauer, C.; Bellotti, E.; Belogurov, S.; Bettini, A.; Bezrukov, L.; Biancacci, V.; Bossio, E.; Bothe, V.; Brudanin, V.; Brugnera, R.; Caldwell, A.; Cattadori, C.; Chernogorov, A.; Comellato, T.; D'Andrea, V.; Demidova, E. V.; Di Marco, N.; Doroshkevich, E.; Fischer, F.; Fomina, M.; Gangapshev, A.; Garfagnini, A.; Gooch, C.; Grabmayr, P.; Gurentsov, V.; Gusev, K.; Hakenmuller, J.; Hemmer, S.; Hofmann, W.; Huang, J.; Hult, M.; Inzhechik, L. V.; Csathy, J. J.; Jochum, J.; Junker, M.; Kazalov, V.; Kermaidic, Y.; Khushbakht, H.; Kihm, T.; Kirpichnikov, I. V.; Klimenko, A.; Kneissl, R.; Knopfle, K. T.; Kochetov, O.; Kornoukhov, V. N.; Krause, P.; Kuzminov, V. V.; Laubenstein, M.; Lindner, M.; Lippi, I.; Lubashevskiy, A.; Lubsandorzhiev, B.; Lutter, G.; Macolino, C.; Majorovits, B.; Maneschg, W.; Manzanillas, L.; Miloradovic, M.; Mingazheva, R.; Misiaszek, M.; Moseev, P.; Muller, Y.; Nemchenok, I.; Pandola, L.; Pelczar, K.; Pertoldi, L.; Piseri, P.; Pullia, A.; Ransom, C.; Rauscher, L.; Riboldi, S.; Rumyantseva, N.; Sada, C.; Salamida, F.; Schonert, S.; Schreiner, J.; Schutt, M.; Schutz, A. K.; Schulz, O.; Schwarz, M.; Schwingenheuer, B.; Selivanenko, O.; Shevchik, E.; Shirchenko, M.; Shtembari, L.; Simgen, H.; Smolnikov, A.; Stukov, D.; Vasenko, A. A.; Veresnikova, A.; Vignoli, C.; von Sturm, K.; Wester, T.; Wiesinger, C.; Wojcik, M.; Yanovich, E.; Zatschler, B.; Zhitnikov, I.; Zhukov, S. V.; Zinatulina, D.; Zschocke, A.; Zsigmond, A. J.; Zuber, K.; Zuzel, G.; Gerda, C., *Characterization of inverted coaxial Ge-76 detectors in GERDA for future double-beta decay experiments.* European Physical Journal C; **81** (2021), 505.

Arutyunov, N.; Krause-Rehberg, R.; Elsayed, M.; Emtsev, V.; Abrosimov, N.; Oganesyan, G.; Kozlovski, V., *Microstructure of bismuth centers in silicon before and after irradiation with 15 MeV protons.* Journal of Physics-Condensed Matter; **33** (2021), 245702.

Publications

Badtke, M.; Tanaka, H.; Ollenburg, L. J.; Kalusniak, S.; Kränkel, C., *Passively Q-switched 8.5-ns* Pr^{3+}*:YLF laser at 640 nm.* Applied Physics B-Lasers and Optics; **127** (2021), 83.

Bae, J. E.; Choi, S. Y.; Kränkel, C.; Hasse, K.; Rotermund, F., *Evanescent-field Q-switched Yb:YAG Channel Waveguide Lasers with Single- and Double-pass Pumping.* Current Optics and Photonics; **5** (2021), 180-185.

Baki, A.; Stöver, J.; Schulz, T.; Markurt, T.; Amari, H.; Richter, C.; Martin, J.; Irmscher, K.; Albrecht, M.; Schwarzkopf, J., *Influence of Sr deficiency on structural and electrical properties of* $SrTiO_3$ *thin films grown by metal-organic vapor phase epitaxy.* Scientific Reports; **11** (2021), 7497.

Barbalas, D.; Chatterjee, S.; Schlom, D. G.; Shen, K. M.; Armitage, N. P., *THz electrodynamics of mixed-valent* $YbAl_3$ *and* $LuAl_3$ *thin films.* European Physical Journal B; **94** (2021), 186.

Barone, M. R.; Dawley, N. M.; Nair, H. P.; Goodge, B. H.; Holtz, M. E.; Soukiassian, A.; Fleck, E. E.; Lee, K.; Jia, Y.; Heeg, T.; Gatt, R.; Nie, Y. F.; Muller, D. A.; Kourkoutis, L. F.; Schlom, D. G., *Improved control of atomic layering in perovskite-related homologous series.* Apl Materials; **9** (2021), 021118.

Bin Anooz, S.; Grüneberg, R.; Chou, T. S.; Fiedler, A.; Irmscher, K.; Wouters, C.; Schewski, R.; Albrecht, M.; Galazka, Z.; Miller, W.; Schwarzkopf, J.; Popp, A., *Impact of chamber pressure and Si-doping on the surface morphology and electrical properties of homoepitaxial (100) beta-*Ga_2O_3 *thin films grown by MOVPE.* Journal of Physics D-Applied Physics; **54** (2021), 034003.

Brewer, A.; Lindemann, S.; Wang, B.; Maeng, W.; Frederick, J.; Li, F.; Choi, Y.; Thompson, P. J.; Kim, J. W.; Mooney, T.; Vaithyanathan, V.; Schlom, D. G.; Rzchowski, M. S.; Chen, L. Q.; Ryan, P. J.; Eom, C. B., *Microscopic piezoelectric behavior of clamped and membrane (001) PMN-30PT thin films.* Applied Physics Letters; **119** (2021), 202903.

Bugallo, D.; Langenberg, E.; Ferreiro-Vila, E.; Smith, E. H.; Stefani, C.; Batlle, X.; Catalan, G.; Domingo, N.; Schlom, D. G.; Rivadulla, F., *Deconvolution of Phonon Scattering by Ferroelectric Domain Walls and Point Defects in a* $PbTiO_3$ *Thin Film Deposited in a Composition-Spread Geometry.* Acs Applied Materials & Interfaces; **13** (2021), 45679-45685.

Cancellara, L.; Markurt, T.; Schulz, T.; Albrecht, M.; Hagedorn, S.; Walde, S.; Weyers, M.; Washiyama, S.; Collazo, R.; Sitar, Z., *Role of oxygen diffusion in the dislocation reduction of epitaxial AlN on sapphire during high-temperature annealing.* Journal of Applied Physics; **130** (2021), 203101.

Chen, Z.; Jiang, Y.; Shao, Y. T.; Holtz, M. E.; Odstrcil, M.; Guizar-Sicairos, M.; Hanke, I.; Ganschow, S.; Schlom, D. G.; Muller, D. A., *Electron ptychography achieves atomic-resolution limits set by lattice vibrations.* Science; **372** (2021), 826-+abg2533.

Chou, T.S., Seyidov, P., Bin Anooz, S., Grüneberg, R., Thi Thuy Vi, T., Irmscher, K., Albrecht, M., Galazka, Z., Schwarzkopf, J., Popp, A., *Fast homoepitaxial growth of (100)* β*-*Ga_2O_3 *thin films via MOVPE,* AIP Advances **11** (2021) 115323

Dawley, N. M.; Pek, E. K.; Lee, C. H.; Ragasa, E. J.; Xiong, X.; Lee, K.; Phillpot, S. R.; Chernatynskiy, A. V.; Cahill, D. G.; Schlom, D. G., *Thermal conductivity of the n=1-5 and 10 members of the* $(SrTiO_3)_{(n)}SrO$ *Ruddlesden-Popper superlattices.* Applied Physics Letters; **118** (2021), 091904.

De Guzman, J. A. T.; Markevich, V. P.; Hawkins, I. D.; Ayedh, H. M.; Coutinho, J.; Binns, J.; Falster, R.; Abrosimov, N. V.; Crowe, I. F.; Halsall, M. P.; Peaker, A. R., *Indium-Doped Silicon for Solar Cells-Light-Induced Degradation and Deep-Level Traps.* Physica Status Solidi a-Applications and Materials Science; **218** (2021), 2100108.

de Guzman, J. A. T.; Markevich, V. P.; Hawkins, I. D.; Coutinho, J.; Ayedh, H. M.; Binns, J.; Abrosimov, N. V.; Lastovskii, S. B.; Crowe, I. F.; Halsall, M. P.; Peaker, A. R., *Acceptor-oxygen defects in silicon: The electronic properties of centers formed by boron, gallium, indium, and aluminum interactions with the oxygen dimer.* Journal of Applied Physics; **130** (2021), 245703.

Derenzo, S.; Bourret, E.; Frank-Rotsch, C.; Hanrahan, S.; Garcia-Sciveres, M., *How silicon and boron dopants govern the cryogenic scintillation properties of N-type GaAs.* Nuclear Instruments & Methods in Physics Research Section a-Accelerators Spectrometers Detectors and Associated Equipment; **989** (2021), 164957.

Dessmann, N.; Le, N. H.; Eless, V.; Chick, S.; Saeedi, K.; Perez-Delgado, A.; Pavlov, S. G.; van der Meer, A. F. G.; Litvinenko, K. L.; Galbraith, I.; Abrosimov, N. V.; Riemann, H.; Pidgeon, C. R.; Aeppli, G.; Redlich, B.; Murdin, B. N., *Highly efficient THz four-wave mixing in doped silicon.* Light-Science & Applications; **10** (2021), 71.

Dey, K.; Ahad, A.; Gautam, K.; Tripathy, A.; Majid, S. S.; Francoual, S.; Richter, C.; Singh, M. N.; Sagdeo, A.; Welter, E.; Vittayakorn, N.; Sathe, V. G.; Rawat, R.; Shukla, D. K., *Coexistence of local structural heterogeneities and long-range ferroelectricity in Pb-free (1-x)*$Ba(Zr_{0.2}Ti_{0.8})O_3$*-x* $(Ba_{0.7}Ca_{0.3})TiO_3$ *ceramics.* Physical Review B; **103** (2021), L100205.

Publications

Dropka, N.; Böttcher, K.; Holena, M., *Development and Optimization of VGF-GaAs Crystal Growth Process Using Data Mining and Machine Learning Techniques.* Crystals; **11** (2021), 1218.

Dropka, N.; Ecklebe, S.; Holena, M., *Real Time Predictions of VGF-GaAs Growth Dynamics by LSTM Neural Networks.* Crystals; **11** (2021), 138.

Drozdowski, W.; Makowski, M.; Witkowski, M. E.; Wojtowicz, A. J.; Irmscher, K.; Schewski, R.; Galazka, Z., *Recent progress in the development of beta-*Ga_2O_3 *scintillator crystals grown by the Czochralski method.* Optical Materials Express; **11** (2021), 2488-2494.

Ernst, O., Uebel, D., Kayser, S., Lange, F., Teuber, T., Boeck, T., *Revealing all states of dewetting of a thin gold layer on a silicon surface by nanosecond laser conditioning.* Applied Surface Science Advances **3** (2021) 100040.

Fajardo, G. J. P.; Howard, S. A.; Evlyukhin, E.; Wahila, M. J.; Mondal, W. R.; Zuba, M.; Boschker, J. E.; Paik, H.; Schlom, D. G.; Sadowski, J. T.; Tenney, S. A.; Reinhart, B.; Lee, W. C.; Piper, L. F. J., *Structural Phase Transitions of* NbO_2*: Bulk versus Surface.* Chemistry of Materials; **33** (2021), 1416-1425.

Fang, Y. W.; Nair, H. P.; Miao, L. D.; Goodge, B.; Schreiber, N. J.; Ruf, J. P.; Kourkoutis, L. F.; Shen, K. M.; Schlom, D. G.; Ramshaw, B. J., *Quantum oscillations and quasiparticle properties of thin film* Sr_2RuO_4. Physical Review B; **104** (2021), 045152.

Fielitz, P.; Ganschow, S.; Kelm, K.; Borchardt, G., *Self-diffusion in high-purity alpha-Al2O3: Comparison of Ti-doped, Mg-doped and undoped single crystals.* Journal of the European Ceramic Society; **41** (2021), 663-668.

Firdous, R.; Hirsch, T.; Klimm, D.; Lothenbach, B.; Stephan, D., *Reaction of calcium carbonate minerals in sodium silicate solution and its role in alkali-activated systems.* Minerals Engineering; **165** (2021), 106849.

Flesch, J.; Bettenhausen, M.; Kazmierczak, M.; Klesse, W. M.; Skibitzki, O.; Psathaki, O. E.; Kurre, R.; Capellini, G.; Guha, S.; Schroeder, T.; Witzigmann, B.; You, C. J.; Piehler, J., *Three-Dimensional Interfacing of Cells with Hierarchical Silicon Nano/Microstructures for Midinfrared Interrogation of In Situ Captured Proteins.* Acs Applied Materials & Interfaces; **13** (2021), 8049-8059.

Frazer, T. D.; Zhu, Y.; Cai, Z. H.; Walko, D. A.; Adamo, C.; Schlom, D. G.; Fullerton, E. E.; Evans, P. G.; Hruszkewycz, S. O.; Cao, Y.; Wen, H. D., *Optical transient grating pumped X-ray diffraction microscopy for studying mesoscale structural dynamics.* Scientific Reports; **11** (2021), 19322.

Galazka, Z.; Ganschow, S.; Irmscher, K.; Klimm, D.; Albrecht, M.; Schewski, R.; Pietsch, M.; Schulz, T.; Dittmar, A.; Kwasniewski, A.; Grueneberg, R.; Bin Anooz, S.; Popp, A.; Juda, U.; Hanke, I. M.; Schroeder, T.; Bickermann, M., *Bulk single crystals of beta-*Ga_2O_3 *and Ga-based spinels as ultra-wide bandgap transparent semiconducting oxides.* Progress in Crystal Growth and Characterization of Materials; **67** (2021), 100511.

Galazka, Z.; Irmscher, K.; Ganschow, S.; Zupancic, M.; Aggoune, W.; Draxl, C.; Albrecht, M.; Klimm, D.; Kwasniewski, A.; Schulz, T.; Pietsch, M.; Dittmar, A.; Grueneberg, R.; Juda, U.; Schewski, R.; Bergmann, S.; Cho, H.; Char, K.; Schroeder, T.; Bickermann, M., *Melt Growth and Physical Properties of Bulk* $LaInO_3$ *Single Crystals.* Physica Status Solidi a-Applications and Materials Science; **218** (2021), 2100016.

Galazka, Z.; Irmscher, K.; Pietsch, M.; Ganschow, S.; Schulz, D.; Klimm, D.; Hanke, I.M.; Schroeder, T.; Bickermann, M., *Experimental Hall electron mobility of bulk single crystals of transparent semiconducting oxides*. Journal of Materials Research **36** (2021) 4746–4755.

Gamov, I.; Hartmann, C.; Straubinger, T.; Bickermann, M., *Photochromism and influence of point defect charge states on optical absorption in aluminum nitride (AlN).* Journal of Applied Physics; **129** (2021), 113103.

Gogolin, M.; Murshed, M. M.; Bayarjargal, L.; Klimm, D.; Gesing, T. M., *Thermal anomalies and phase transitions in* $Pb_2Sc_2Si_2O_9$ *and* $Pb_2In_2Si_2O_9$. Zeitschrift Fur Kristallographie-Crystalline Materials; **236** (2021), 283-292.

Gradwohl, K. P.; Juda, U.; Sumathi, R. R., *The impact of the dislocation distribution and dislocation type on the charge carrier lifetime in Czochralski germanium single crystals.* Journal of Crystal Growth; **573** (2021), 126285.

Gradwohl, K. P.; Roder, M.; Danilewsky, A. N.; Sumathi, R. R., *Investigation of the dislocation structure in Czochralski germanium crystals grown in 211 and 110 growth directions.* Crystengcomm; **23** (2021), 4116-4124.

Gunes, M.; Donmez, O.; Gumus, C.; Erol, A.; Alghamdi, H.; Alhassan, S.; Alhassni, A.; Alotaibi, S.; Schmidbauer, M.; Galeti, H. V. A.; Henini, M., *The effect of strain and spatial Bi distribution on the band alignment of GaAsBi single quantum well structure.* Physica B-Condensed Matter; **602** (2021), 412487.

Guzman, de J. A. T.; Markevich,V. P.; Coutinho, J.; Abrosimov, N. V.; Halsall, M. P.; and Peaker, A. R., *Electronic Properties and Structure of Boron–Hydrogen Complexes in Crystalline Silicon*, Sol. RRL 2021, 2100459

Publications

Haase, P.; Christensen, H. G.; Nielsen, U. G.; Koch, C. B.; Galazka, Z., Majzlan, J., *Stability and solubility of members of tin perovskites in the schoenfliesite subgroup,* $_2(BSn^{4+})(OH,O)_6$ *(B = Ca,* Fe^{3+}*, Mg,* Mn^{2+}*, Zn, Cu).* Chemical Thermodynamics and Thermal Analysis; **1-2** (2021), 100005.

Hagedorn, S.; Mogilatenko, A.; Walde, S.; Pacak, D.; Weinrich, J.; Hartmann, C.; Weyers, M., *High-Temperature Annealing and Patterned AlN/Sapphire Interfaces.* Physica Status Solidi B-Basic Solid State Physics; **258** (2021), 2100187.

Hasse, K.; Kip, D.; Kränkel, C., *Influence of diluted acid mixtures on selective etching of MHz- and kHz-fs-laser inscribed structures in YAG.* Optical Materials Express; **11** (2021), 1546-1554.

Held, R.; Mundy, J. A.; Holtz, M. E.; Hodash, D.; Mairoser, T.; Muller, D. A.; Schlom, D. G., *Fabrication of chemically and structurally abrupt Eu1-xLaxO/SrO/Si interfaces and their analysis by STEM-EELS.* Physical Review Materials; **5** (2021), 124419.

Hensling, F. V. E.; Dahliah, D.; Dulal, P.; Singleton, P.; Sun, J. X.; Schubert, J.; Paik, H. J.; Subedi, I.; Subedi, B.; Rignanese, G. M.; Podraza, N. J.; Hautier, G.; Schlom, D. G., *Epitaxial stannate pyrochlore thin films: Limitations of cation stoichiometry and electron doping.* Apl Materials; **9** (2021), 051113.

Hilfiker, M.; Stokey, M.; Korlacki, R.; Kilic, U.; Galazka, Z.; Irmscher, K.; Zollner, S.; Schubert, M., *Zinc gallate spinel dielectric function, band-to-band transitions, and Gamma-point effective mass parameters.* Applied Physics Letters; **118** (2021), 132102.

Hirschle, C.; Schreuer, J.; Galazka, Z.; Ritter, C., *On the relation of structural disorder and thermoelastic properties in* $ZnGa_2O_4$ *and* $Zn_{1-x}MgxGa_2O_4$ *(x approximate to 0.33).* Journal of Alloys and Compounds; **886** (2021), 161214.

Holtz, M. E.; Padgett, E. S.; Steinhardt, R.; Brooks, C. M.; Meier, D.; Schlom, D. G.; Muller, D. A.; Mundy, J. A., *Dimensionality-Induced Change in Topological Order in Multiferroic Oxide Superlattices.* Physical Review Letters; **126** (2021), 157601.

Hu, Y. Q.; Yao, X. L.; Schlom, D. G.; Datta, S.; Cho, K., *First Principles Design of High Hole Mobility p-Type Sn-O-X Ternary Oxides: Valence Orbital Engineering of* Sn^{2+} *in* Sn^{2+}*-O-X by Selection of Appropriate Elements X.* Chemistry of Materials; **33** (2021), 212-225.

Huyan, H.; Addiego, C.; Yan, X. X.; Gadre, C. A.; Melville, A.; Schlom, D. G.; Pan, X. Q., *Direct observation of polarization-induced two-dimensional electron/hole gases at ferroelectric-insulator interface.* Npj Quantum Materials; **6** (2021), 88.

Kayser, S.; Rotundo, N.; Dropka, N.; Farrell, P., *Assessing doping inhomogeneities in GaAs crystal via simulations of lateral photovoltage scanning method.* Journal of Crystal Growth; **571** (2021), 126248.

Khirunenko, L.; Sosnin, M.; Duvanskii, A.; Abrosimov, N.; Riemann, H., *The Features of Infrared Absorption of Boron-Doped Silicon.* Physica Status Solidi a-Applications and Materials Science; **218** (2021), 2100181.

Kim, H.; Lu, K. Y.; Liu, Y. P.; Kum, H. S.; Kim, K. S.; Qiao, K.; Bae, S. H.; Lee, S.; Ji, Y. J.; Kim, K. H.; Paik, H.; Xie, S. E.; Shin, H.; Choi, C.; Lee, J. H.; Dong, C. Y.; Robinson, J. A.; Lee, J. H.; Ahn, J. H.; Yeom, G. Y.; Schlom, D. G.; Kim, J., *Impact of 2D-3D Heterointerface on Remote Epitaxial Interaction through Graphene.* Acs Nano; **15** (2021), 10587-10596.

Kränkel, C.; Uvarova, A.; Haurat, E.; Hulshoff, L.; Brutzam, M.; Guguschev, C.; Kalusniak, S.; Klimm, D., *Czochralski growth of mixed cubic sesquioxide crystals in the ternary system* Lu_2O_{3}*-*Sc_2O_{3}*-*Y_2O_3*.* Acta Crystallographica Section B-Structural Science Crystal Engineering and Materials; **77** (2021), 550-558.

Kurajica, S.; Sipusic, J.; Zupancic, M.; Brautovic, I.; Albrecht, M., $ZnO\text{-}Al_2O_3\text{-}SiO_2$ *glass ceramics: Influence of composition on crystal phases, crystallite size and appearance.* Journal of Non-Crystalline Solids; **553** (2021), 120481.

Lavrov, E. V.; Melnikov, V. V.; Abrosimov, N. V., *Interstitial* H_2 *in* ^{29}Si*.* Physical Review B; **103** (2021), 205204.

Liang, S. J.; Finck, D.; Neis, M. W.; Schwarzkopf, J.; Mayer, D.; Wordenweber, R., *SAW gas sensor based on extremely thin strain-engineered* $K_{0.7}Na_{0.3}NbO_3$ *films.* Applied Physics Letters; **119** (2021), 112905.

Liang, Y. Y.; Qiao, W. C.; Feng, T. L.; Zhang, B. T.; Zhao, Y. F.; Song, Y. Z.; Li, T.; Krankel, C., *Investigation on the optical nonlinearity of the layered magnesium-mediated metal organic framework (Mg-MOF-74).* Optics Express; **29** (2021), 23786-23798.

Litvinenko, K. L.; Le, N. H.; Redlich, B.; Pidgeon, C. R.; Abrosimov, N. V.; Andreev, Y.; Huang, Z. M.; Murdin, B. N., *The multi-photon induced Fano effect.* Nature Communications; **12** (2021), 454.

Publications

Lyle, L. A. M.; Jiang, K. Y.; Favela, E. V.; Das, K.; Popp, A.; Galazka, Z.; Wagner, G.; Porter, L. M., *Effect of metal contacts on (100) beta-Ga_2O_3 Schottky barriers.* Journal of Vacuum Science & Technology A; **39** (2021), 033202.

McCandless, J. P.; Chang, C. S.; Nomoto, K.; Casamento, J.; Protasenko, V.; Vogt, P.; Rowe, D.; Gann, K.; Ho, S. T.; Li, W.; Jinno, R.; Cho, Y.; Green, A. J.; Chabak, K. D.; Schlom, D. G.; Thompson, M. O.; Muller, D. A.; Xing, H. G.; Jena, D., *Thermal stability of epitaxial alpha-Ga_2O_3 and (Al,Ga)$_2$O$_3$ layers on m-plane sapphire.* Applied Physics Letters; **119** (2021), 062102.

McQuade, G. A.; Plaut, A. S.; Usher, A.; Martin, J., *The thermal expansion coefficient of monolayer, bilayer, and trilayer graphene derived from the strain induced by cooling to cryogenic temperatures.* Applied Physics Letters; **118** (2021), 203101.

Meisenheimer, P. B.; Steinhardt, R. A.; Sung, S. H.; Williams, L. D.; Zhuang, S.; Nowakowski, M. E.; Novakov, S.; Torunbalci, M. M.; Prasad, B.; Zollner, C. J.; Wang, Z.; Dawley, N. M.; Schubert, J.; Hunter, A. H.; Manipatruni, S.; Nikonov, D. E.; Young, I. A.; Chen, L. Q.; Bokor, J.; Bhave, S. A.; Ramesh, R.; Hu, J. M.; Kioupakis, E.; Hovden, R.; Schlom, D. G.; Heron, J. T., *Engineering new limits to magnetostriction through metastability in iron-gallium alloys.* Nature Communications; **12** (2021), 2757.

Nascimento, V. M.; Mechin, L.; Liu, S.; Aryan, A.; Adamo, C.; Schlom, D. G.; Guillet, B., *Electro-thermal and optical characterization of an uncooled suspended bolometer based on an epitaxial $La_{0.7}Sr_{0.3}MnO_3$ film grown on $CaTiO_3$/ Si.* Journal of Physics D-Applied Physics; **54** (2021), 055301.

Nentwich, M.; Weigel, T.; Richter, C.; Stocker, H.; Mehner, E.; Jachalke, S.; Novikov, D. V.; Zschornak, M.; Meyer, D. C., *Sample chamber for synchrotron based in-situ X-ray diffraction experiments under electric fields and temperatures between 100 K and 1250 K.* Journal of Synchrotron Radiation; **28** (2021), 158-168.

Noatschk, K.; Hofmann, E. V. S.; Dabrowski, J.; Curson, N. J.; Schroeder, T.; Klesse, W. M.; Seibold, G., *Ge(001) surface reconstruction with Sn impurities.* Surface Science; **713** (2021), 121912.

Pavlov, S. G.; Astrov, Y. A.; Portsel, L. M.; Shuman, V. B.; Lodygin, A. N.; Abrosimov, N. V.; Hubers, H. W., *Magnesium-related shallow donor centers in silicon.* Materials Science in Semiconductor Processing; **130** (2021), 105833.

Pavlov, S. G.; Portsel, L. M.; Shuman, V. B.; Lodygin, A. N.; Astrov, Y. A.; Abrosimov, N. V.; Lynch, S. A.; Tsyplenkov, V. V.; Hubers, H. W., *Infrared absorption cross sections, and oscillator strengths of interstitial and substitutional double donors in silicon.* Physical Review Materials; **5** (2021), 114607.

Pavlov, S. G.; Prikhodko, D. D.; Tarelkin, S. A.; Bormashov, V. S.; Abrosimov, N. V.; Kuznetsov, M. S.; Terentiev, S. A.; Nosukhin, S. A.; Troschiev, S. Y.; Blank, V. D.; Hubers, H. W., *Resonant boron acceptor states in semiconducting diamond.* Physical Review B; **104** (2021), 155201.

Pfutzenreuter, D.; Zupancic, M.; Galazka, Z.; Schewski, R.; Dittmar, A.; Irmscher, K.; Albrecht, M.; Schwarzkopf, J., *Epitaxial $BaSnO_3$ thin films with low dislocation density grown on lattice matched $LaInO_3$ substrates.* Nanotechnology; **32** (2021), 505609.

Porz, L.; Knez, D.; Scherer, M.; Ganschow, S.; Kothleitner, G.; Rettenwander, D., *Dislocations in ceramic electrolytes for solid-state Li batteries.* Scientific Reports; **11** (2021), 8949.

Puschel, S.; Kalusniak, S.; Krankel, C.; Tanaka, H., *Temperature-dependent radiative lifetime of Yb:YLF: refined cross sections and potential for laser cooling.* Optics Express; **29** (2021), 11106-11120.

Redhammer, G. J.; Badami, P.; Meven, M.; Ganschow, S.; Berendts, S.; Tippelt, G.; Rettenwander, D., *Wet-Environment-Induced Structural Alterations in Single- and Polycrystalline LLZTO Solid Electrolytes Studied by Diffraction Techniques.* Acs Applied Materials & Interfaces; **13** (2021), 350-359.

Redhammer, G. J.; Meven, M.; Ganschow, S.; Tippelt, G.; Rettenwander, D., *Single-crystal neutron and X-ray diffraction study of garnet-type solid-state electrolyte $Li_6La_3ZrTaO_{12}$: an in situ temperature-dependence investigation (2.5 <= T <= 873 K).* Acta Crystallographica Section B-Structural Science Crystal Engineering and Materials; **77** (2021), 123-130.

Regmi, S.; Li, Z.; Srivastava, A.; Mahat, R.; Kc, S.; Rastogi, A.; Galazka, Z.; Datta, R.; Mewes, T.; Gupta, A., *Structural and magnetic properties of $NiFe_2O_4$ thin films grown on isostructural lattice-matched substrates.* Applied Physics Letters; **118** (2021), 152402.

Reichmann,F.; Dabrowski, J.; Becker, A. P.; Klesse, W. M.; Irmscher, K.; Schewski, R.; Galazka, Z.; Mulazzi M.; *Experimental and Theoretical Investigation of the Surface Electronic Structure of ZnGa2O4 (100) Single Crystals*, Phys. Status Solidi B 259 (2021) 2100452.

Publications

Rodenbucher, C.; Guguschev, C.; Korte, C.; Bette, S.; Szot, K., *Is Reduced Strontium Titanate a Semiconductor or a Metal?* Crystals; **11** (2021), 744.

Ruf, J. P.; Paik, H.; Schreiber, N. J.; Nair, H. P.; Miao, L.; Kawasaki, J. K.; Nelson, J. N.; Faeth, B. D.; Lee, Y.; Goodge, B. H.; Pamuk, B.; Fennie, C. J.; Kourkoutis, L. F.; Schlom, D. G.; Shen, K. M., *Strain-stabilized superconductivity.* Nature Communications; **12** (2021), 59.

Sauter, E., Abrosimov, N.V., Hübner J., Oestreich, M., *Low temperature relaxation of donor bound electron spins in ^{28}Si:P.* Phys. Rev. Lett. **126** (2021) 137402

Schmidt, D.; Bauer, R.; Chung, S.; Novikov, D.; Sander, M.; Pudell, J. E.; Herzog, M.; Pfuetzenreuter, D.; Schwarzkopf, J.; Chernikov, R.; Gaal, P., *A new concept for temporal gating of synchrotron X-ray pulses.* Journal of Synchrotron Radiation; **28** (2021), 375-382.

Smalc-Koziorowska, J.; Grzanka, E.; Lachowski, A.; Hrytsak, R.; Grabowski, M.; Grzanka, S.; Kret, S.; Czernecki, R.; Turski, H.; Marona, L.; Markurt, T.; Schulz, T.; Albrecht, M.; Leszczynski, M., *Role of Metal Vacancies in the Mechanism of Thermal Degradation of InGaN Quantum Wells.* Acs Applied Materials & Interfaces; **13** (2021), 7476-7484.

Smetaczek, S.; Pycha, E.; Ring, J.; Siebenhofer, M.; Ganschow, S.; Berendts, S.; Nenning, A.; Kubicek, M.; Rettenwander, D.; Limbeck, A.; Fleig, J., *Investigating the electrochemical stability of $Li_7La_3Zr_2O_{12}$ solid electrolytes using field stress experiments.* Journal of Materials Chemistry A; **9** (2021), 15226-15237.

Steinhardt, R. A.; Brooks, C. M.; Correa, G. C.; Holtz, M. E.; Ramesh, R.; Muller, D. A.; Mundy, J. A.; Schlom, D. G., *$DyFe_2O_4$: A new trigonal rare-earth ferrite grown by molecular-beam epitaxy.* Apl Materials; **9** (2021), 041106.

Stokey, M.; Korlacki, R.; Knight, S.; Ruder, A.; Hilfiker, M.; Galazka, Z.; Irmscher, K.; Zhang, Y. X.; Zhao, H. P.; Darakchieva, V.; Schubert, M., *Optical phonon modes, static and high-frequency dielectric constants, and effective electron mass parameter in cubic In_2O_3.* Journal of Applied Physics; **129** (2021), 225102.

Suhak, Y.; Roshchupkin, D.; Redkin, B.; Kabir, A.; Jerliu, B.; Ganschow, S.; Fritze, H., *Correlation of Electrical Properties and Acoustic Loss in Single Crystalline Lithium Niobate-Tantalate Solid Solutions at Elevated Temperatures.* Crystals; **11** (2021), 398.

Suyolcu, Y. E.; Sun, J. X.; Goodge, B. H.; Park, J.; Schubert, J.; Kourkoutis, L. F.; Schlom, D. G., *a-axis $YBa_2Cu_3O_{7-x}$/$PrBa_2Cu_3O_{7-x}$/$YBa_2Cu_3O_{7-x}$ trilayers with subnanometer rms roughness.* Apl Materials; **9** (2021), 021117.

Suzuki, A.; Kränkel, C.; Tokurakawa, M., *Sub-6 optical-cycle Kerr-lens mode-locked $Tm:Lu_2O_3$ and $Tm:Sc_2O_3$ combined gain media laser at 2.1 mu m.* Optics Express; **29** (2021), 19465-19471.

Talantsev, E. F.; Stolze, K., *Resistive transition of hydrogen-rich superconductors.* Superconductor Science & Technology; **34** (2021), 064001.

Tokurakawa, M., Suzuki, A., Kränkel, C., *Kerr-lens mode-locked Tm solid state laser with spectral broadening effect*. Rev. Las. Eng. 49 (7) (2021) 385.

Uhlendorf, J.; Galazka, Z.; Schmidt, H., *Oxygen diffusion in beta-Ga_2O_3 single crystals at high temperatures.* Applied Physics Letters; **119** (2021), 242106.

Vogt, P.; Hensling, F. V. E.; Azizie, K.; Chang, C. S.; Turner, D.; Park, J.; McCandless, J. P.; Paik, H.; Bocklund, B. J.; Hoffman, G.; Bierwagen, O.; Jena, D.; Xing, H. L. G.; Mou, S.; Muller, D. A.; Shang, S. L.; Liu, Z. K.; Schlom, D. G., *Adsorption-controlled growth of Ga_2O_3 by suboxide molecular-beam epitaxy.* Apl Materials; **9** (2021), 031101.

Vogt, P.; Hensling, F. V. E.; Azizie, K.; Chang, C. S.; Turner, D.; Park, J.; McCandless, J. P.; Paik, H.; Bocklund, B. J.; Hoffmann, G.; Bierwagen, O.; Jena, D.; Xing, H. L. G.; Mou, S.; Muller, D. A.; Shang, S. L.; Liu, Z. K.; Schlom, D. G., *Adsorption-controlled growth of Ga_2O_3 by suboxide molecular-beam epitaxy (vol 9, 031101, 2021).* Apl Materials; **9** (2021), 049901.

Wan, G.; Freeland, J. W.; Kloppenburg, J.; Petretto, G.; Nelson, J. N.; Kuo, D. Y.; Sun, C. J.; Wen, J. G.; Diulus, J. T.; Herman, G. S.; Dong, Y. Q.; Kou, R. H.; Sun, J. Y.; Chen, S.; Shen, K. M.; Schlom, D. G.; Rignanese, G. M.; Hautier, G.; Fong, D. D.; Feng, Z. X.; Zhou, H.; Suntivich, J., *Amorphization mechanism of $SrIrO_3$ electrocatalyst: How oxygen redox initiates ionic diffusion and structural reorganization.* Science Advances; **7** (2021), eabc7323.

Wang, Y. C.; Nair, H. P.; Schreiber, N. J.; Ruf, J. P.; Cheng, B.; Schlom, D. G.; Shen, K. M.; Armitage, N. P., *Separated transport relaxation scales and interband scattering in thin films of $SrRuO_3$, $CaRuO_3$, and Sr_2RuO_4.* Physical Review B; **103** (2021), 205109.

Winkler, R. S.; Zhang, Y. Y.; Zhang, Q.; Wang, Z.; Zhu, Y. M.; Han, M. G.; Schlom, D. G.; Valanoor, N., *Electromechanical Manipulation of Topological Defects to Yield Giant Piezoelectric Response in Epitaxial Lead Zirconate Titanate Bilayers on Silicon.* Advanced Electronic Materials; **7** (2021), 2100195.

Wolff, N.; Klimm, D.; Habicht, K.; Fritsch, K., *Crystal growth and thermodynamic investigation of $Bi_2M^{2+}O_4$ (M = Pd, Cu).* Crystengcomm; **23** (2021), 3230-3238.

Publications

Xu, L. C.; Fauque, B.; Zhu, Z. W.; Galazka, Z.; Irmscher, K.; Behnia, K., *Thermal conductivity of bulk* In_2O_3 *single crystals.* Physical Review Materials; **5** (2021), 014603.

Yan, X. X.; Liu, C. Y.; Gadre, C. A.; Gu, L.; Aoki, T.; Lovejoy, T. C.; Dellby, N.; Krivanek, O. L.; Schlom, D. G.; Wu, R. Q.; Pan, X. Q., *Single-defect phonons imaged by electron microscopy.* Nature; **589** (2021), 65-+.

Zeuschner, S. P.; Mattern, M.; Pudell, J. E.; von Reppert, A.; Rossle, M.; Leitenberger, W.; Schwarzkopf, J.; Boschker, J. E.; Herzog, M.; Bargheer, M., *Reciprocal space slicing: A time-efficient approach to femtosecond x-ray diffraction.* Structural Dynamics-Us; **8** (2021), 014302.

Zheng, X. D.; Gerber, E.; Park, J. S.; Werder, D.; Kigner, O.; Kim, E. A.; Xie, S. E.; Schlom, D. G., *Utilizing complex oxide substrates to control carrier concentration in large-area monolayer* MoS_2 *films.* Applied Physics Letters; **118** (2021), 093103.

Zhou, M. J.; Wang, B.; Ladera, A.; Bogula, L.; Liu, H. X.; Chen, L. Q.; Nan, C. W., *Phase diagrams, superdomains, and superdomain walls in* $K_xNa_{1-x}NbO_3$ *epitaxial thin films.* Acta Materialia; **215** (2021), 117038.

Zimmermann, F.; Beyer, J.; Beyer, F. C.; Gartner, G.; Gamov, I.; Irmscher, K.; Richter, E.; Weyers, M.; Heitmann, J., *A carbon-doping related luminescence band in GaN revealed by below bandgap excitation.* Journal of Applied Physics; **130** (2021), 055703.

Zimmermann, F.; Beyer, J.; Roder, C.; Beyer, F. C.; Richter, E.; Irmscher, K.; Heitmann, J., *Current Status of Carbon-Related Defect Luminescence in GaN.* Physica Status Solidi a-Applications and Materials Science; **218** (2021), 2100235.

Talks

Invited talks at national and international conferences and workshops

N.V. Abrosimov, *Fabrication of* ^{28}Si *for application in quantum computation,* E-MRS Fall Meeting 2021, online

K. Dadzis, A. Enders-Seidlitz, and J. Pal, *Validation of multi-physical models for crystal growth,* presented at the 2nd International Symposium on Modeling of Crystal Growth Processes and Devices (MCGPD-21), Chennai, India (online), July 5-8, 2021.

N. Dropka, M. Holena, *Recent advances and applications of data mining and machine learning in bulk crystal growth*, DKT-2021, Berlin, Germany

N. Dropka, K. Böttcher, M. Holena, *Smart development of vertical gradient freeze crystal growth recipes*, 22nd American Conference on Crystal Growth and Epitaxy (ACCGE-22), USA, online

A. Enders-Seidlitz and K. Dadzis, *pyelmer - Python interface for Elmer workflow,* presented at the Elmer FEM Webinar Series, Espoo, Finland (online), April 29, 2021

Z. Galazka; *Czochralski growth and physical properties of bulk* β-Ga_2O_3 *single crystals*, American Conference on Crystal Growth and Epitaxy (ACCGE-22), USA. Online.

C. Hartmann, T. Schröder, A. Popp, *Recent progress on IKZ wide band gap materials R & D: The examples of AlN &* Ga_2O_3*,* 2021 Semiconductor Novel Materials Development (Taiyuan), online

S. Kalusniak, H. Tanaka, E. Castellano-Hernández, C. Kränkel, *Enhanced absorption efficiency in UV-pumped* Tb^{3+}*: LLF,* The European Conference on Lasers and Electro-Optics 2021, Munich, Germany

C. Kränkel, E. Castellano-Hernández, S. Kalusniak, and H. Tanaka, *Tb-Lasers: Current state and future prospects,* The 10th Advanced Lasers and Photon Sources (ALPS2021), online

J. Martin (& D. Nguyen, A. Yuvanc, T. Schröder, J. Schwarzkopf), *New perspectives on Layer Transfer and Artificial Crystalline Heterostructures*, DKT 21 Deutsche Kristallzüchtungstagung, 6.-8. Oktober 2021

J. Martin, *Electronic structure of 2D-vdWaals materials and heterostructures*, ikz-winterschool 8.-10. 12. 2021

W. Miller, Atomistic Calculations as a Tool to Understand Growth Kinetics in Epitaxial Processes, 2nd International Symposium on Modeling of Crystal Growth Processes and Devices (MCGPD-2021), online

Talks

A. Popp, S. Bin Anooz, T.-S. Chou, R. Grüneberg, K. Irmscher, C. Wouters, R. Schewski, M. Albrecht, Z. Galazka, W. Miller, J. Schwarzkopf, *Homoepitaxial growth of β-Ga_2O_3 by MOVPE on vicinal (100) oriented substrates – influence of growth parameters –* SPIE_Photonics West 2021, San Francisco, USA

A. Popp, S. Bin Anooz, T.-S. Chou, R. Grüneberg, R. Schewski, C. Wouters, A. Fiedler, M. Pietsch, A. Kwasniewski, M. Schmidbauer, W. Miller, Z. Galazka, K. Irmscher, M. Albrecht, J. Schwarzkopf, *Recent progress on IKZ wide band gap materials R & D: The examples of AlN & Ga_2O_3*, 2021 Semiconductor Novel Materials Development (Taiyuan), online

A. Popp, C. Hartmann, T. Schröder, *Recent progress on IKZ wide band gap materials R & D: The examples of AlN & Ga_2O_3*, 2021 Semiconductor Novel Materials Development (Taiyuan), online

M. Schmidbauer, L. Bogula, B. Wang, M. Hanke, L. von Helden, A. Ladera, J.-J. Wang, L.-Q. Chen, J. Schwarzkopf, *Ferroelectric Phase Transitions in Strained $K_{0.9}Na_{0.1}NbO_3$ Epitaxial Films Studied by in situ X-Ray Diffraction and Three-Dimensional Phase-Field Simulations*, AAAFM-UCLA 2021, Advances in Functional Materials, Los Angeles, USA, hybrid conference

R. R. Sumathi, C. Hartmann, T. Straubinger, M. Bickermann, *Hetero-epitaxy and homo-epitaxy for AlN native substrate technology: Challenges & Benefits,* XXI International Workshop on the Physics of Semiconductor Devices (IWPSD 2021), India, online

R. R. Sumathi, K.-P. Gradwohl, A. Gybin, N. Dropka, T. Schröder, S. Schönert, *High-purity Ge crystal growth and its specific use-case application for high-sensitive detection of neutrinoless ßß-decay,* 22nd American Conference on Crystal Growth and Epitaxy (ACCGE-22), USA, online

R. R. Sumathi, K.-P. Gradwohl, A. Gybin, V. I. Lakshmanan, M.A. Halim, *Processing opportunities for electronic-grade Ge: Utilising known recovery and reduction technology improvements,* European Materials Research Society Spring Meeting (E-MRS 2021), online

R. R. Sumathi, R. Menzel, *High purity semiconductor (Si, Ge) crystals: Why are they needed?,* The Third Indian Materials Conclave and the 32nd Annual General Meeting of MRSI, online

T. Schröder, A. Popp, C. Hartmann, *Recent progress on IKZ wide band gap materials R & D: The examples of AlN & Ga_2O_3*, 2021 Semiconductor Novel Materials Development (Taiyuan), online

Invited seminars at national and international institutions

M. Albrecht, *in-situ TEM Aktivitäten & Data Science & FAIRMAT*, BTU CS - IKZ Workshop, Berlin, Germany, 2021

H. Amari, *In-Situ Electron Microscopy research activities at Leibniz-Institut für Kristallzüchtung (IKZ)*, Agenda Workshop IKZ / IOM, Leipzig, Germany

M. Bickermann, *Bulk Crystal Growth for Functional Materials, Using Silicon as an Example,* lecture series at Phillips-Universität Marburg, Germany

N. Dropka, *Recent advances and applications of machine learning in bulk crystal growth*, BR50 Workshop on Artificial Intelligence in Research, Berlin, Germany

N. Dropka, *Simulation und KI in der Kristallzüchtung*, BTU CS-IKZ Workshop, Berlin, Germany

C. Hartmann, *AlN Kristallzüchtung und Nanostrukturierung*, Agenda Workshop IKZ / IOM, Leipzig, Germany

Z. Galazka, *Bulk β-Ga2O3 single crystals – growth by the Czochralski method and physical properties*. Ohio State University, Ohio, USA, 3 June 2021. On-line.

Z. Galazka, *Ultra-wide bandgap oxide semiconductor β-Ga2O3: bulk single crystals, physical properties, and applications.* University of Warsaw, Institute of Physics, Warsaw, Poland, 15 January 2021. On-line.

Y. Goto, T. Schröder, *Interim Closing Remarks*, Leibniz Association – Japan Science and Technology Agency (JST), Online Workshop on Covid-19 Research Collaboration

H. Katayama, T. Kato, T. Schröder, J. Strunk, M. Wächtler, M. Gunzer, *CREST Project – Creative Development for Detection and Removal of Viruses in Environment Using New Materials*, Leibniz Association – Japan Science and Technology Agency (JST) Online Workshop on Covid-19 Research Collaboration

C. Kränkel, *Kristalle für Photonik (Laser, opt. Isolatoren, nichtlineare Optik),* Agenda Workshop IKZ / IOM, Leipzig, Germany

C. Kränkel, *Research activities at the Center for Laser Materials,* Fakultät für Elektrotechnik Experimentalphysik und Materialwissenschaften, Helmut-Schmidt-Universität Hamburg, Germany

A. Popp, *Ga_2O_3 Epitaxie,* BTU CS, IKZ Workshop, Berlin, Germany

A. Popp, *Ga_2O_3 material for vertical power devices: Challenges to the Epitaxy Process*, Agenda Workshop IKZ / IOM, Leipzig, Germany

Talks

A. Popp, *Ga_2O_3 material for vertical power devices: Challenges to the Epitaxy Process*, University Bristol, online

T. Schröder, T. Straubinger, *IKZ: UVC LED & Laserdiode on AlN Substrate for metrology on bacteria and virus,* Leibniz Association and Japan Science and Technology Agency (JST): Online Workshop on Covid-19 Research Collaboration

T. Schröder, *Kurze Institutsvorstellung,* Agenda Workshop IKZ / IOM, Leipzig, Germany

T. Schröder, *Leibniz debattiert – Technologische Souveränität,* Leibniz-Gemeinschaft, Berlin, Germany

T. Schröder, *Technologische Souveränität in der Materialwissenschaft,* Berlin Science Week (Moderator), Berlin, Germany

J. Schwarzkopf, *Impact of lattice strain on structure and electric properties of alkaline-niobate thin films,* Online Seminar Series on Antiferroelectric Materials, TU Darmstadt, Germany

J. Schwarzkopf, A. Baki, D. Pfützenreuter, Y. Wang, S. Bin Anooz, D. A. Nguyen, A. Yuvanc, J. Martin, *Growth of complex metal oxides at IKZ,* BTU CS-IKZ Workshop, Germany

J. Schwarzkopf, *Impact of lattice strain in ferroelectric alkaline niobate thin films,* Leipzig University, seminar: Halbleiterphysik des Felix-Bloch-Institut für Festkörperphysik; Leipzig, Germany

T. Straubinger, *Kristallbearbeitung & Oberflächenbehandlung,* Agenda Workshop IKZ / IOM, Leipzig, Germany

R. R. Sumathi, *Halbleiterkristalle*, Agenda Workshop IKZ / IOM, 4. und 5.10.2021, Leipzig, Germany

S. Zahedi-Azad, *Selektive CVD Nanostrukturen*, BTU CS, IKZ Workshop, Berlin, Germany

Oral contributions at national and international conferences

M. Badtke, H.Tanaka, L. J. Ollenburg, S. Kalusniak, and C. Kränkel, *Sub-10-ns passively Q-switched red Pr:YLF laser,* CLEO, in San Jose, USA

M. Badtke, H. Tanaka, L. Ollenburg, S. Kalusniak, and C. Kränkel, *Miniaturized passively Q-switched Pr:YLF laser,* Conference on Lasers and Electro-Optics (CLEO/Europe-EQEC) 2021, Munich, Germany

K. Dadzis and A. Enders-Seidlitz, *Coupled 3D calculations of fluid flow, heat and mass transport, and phase boundary shape for crystal growth processes,* presented at the 16th OpenFOAM Workshop (OFW16), Dublin, Ireland (online), June 8-11, 2021.

M. Bickermann, M. Schulze, T. Schwaigert, M. Stypa, M. Brützam, S. Ganschow, C. Guguschev, *Substrate Crystals for Advanced Functional Oxides,* 10th German-French Workshop on Oxide, Dielectric, and Laser Single Crystals 2022, Idar-Oberstein, Germany

N. Dropka, A.G. Ostrogorsky, *Interface shape under the insulating baffle in vertical Bridgman systems,* 22nd American Conference on Crystal Growth and Epitaxy (ACCGE-22), USA, online

N. Dropka, J. Fischer, A. Gybin, N. Abrosimov, R. Sumathi, *Numerical optimization of gas management for the growth of high-purity, high-quality germanium single crystals,* 22nd American Conference on Crystal Growth and Epitaxy (ACCGE-22), USA, online

A. Enders-Seidlitz, J. Pal, K. Dadzis, *Development of a python-based crystal growth simulation framework,* 2nd preCICE Workshop, University of Stuttgart, Germany

A. Enders-Seidlitz, J. Pal, and K. Dadzis, *Development of an open-source-based framework for multiphysical crystal growth simulations,* presented at the FEniCS Conference, Cambridge, UK (online), March 22-26, 2021.

A. Enders-Seidlitz, J. Pal, and K. Dadzis, *Experimental and numerical analysis of resistive and inductive heating in CZ growth,* presented at the Deutsche Kristallzüchtungstagung (DKT), Berlin, Germany, October 6-8, 2021.

F. Flatscher, V. Reisecker, S. Ganschow, R. Brunner, Y.-M. Chiang, D. Rettenwander, *Enabling high-rate plating in solid-state Li batteries by interface engineering and pulse plating,* 239th ECS Meeting with the 18th International Meeting on Chemical Sensors (IMCS), Chicago, USA

Talks

K.-P. Gradwohl, M. Roder, A. Danilewsky, R. R. Sumathi, *Dislocation structure of Cz-Ge crystals grown in [110] and [211] direction,* The 8th Asian Conference on Crystal Growth and Crystal Technology, Japan, online

K.-P. Gradwohl, W. Miller, N. Dropka, R.R. Sumathi, *Discrete dislocation dynamics simulations as a tool to derive quantitative dislocation multiplication laws in semiconductor crystals,* Deutsche Kristallzüchtungstagung DKT 2021, Berlin, Germany

K. Hasse, D. Kip, C. E. Rüter, and C. Kränkel, *Selective etching of 10 MHz fs-laser inscribed tracks in YAG,* EOS Annual Meeting (EOSAM) 2021, Rome, Italy

L. Hülshoff, A. Uvarova, C. Guguschev, S. Kalusniak, H. Tanka, D. Klimm, and C. Kränkel, *Czochralski growth and laser operation of Er- and Yb-doped mixed sesquioxide crystals,* Advanced Solid-State Lasers Conference 2021, online

S. Kalusniak, H. Tanaka, E. Castellano-Hernández, and C. Kränkel, *Enhanced absorption efficiency in UV-pumped Tb^{3+}:LLF,* Conference on Lasers and Electro-Optics (CLEO/Europe-EQEC) 2021, Munich, Germany

S. Kalusniak, H. Tanka, E. Castellano-Hernández, and C. Kränkel, *UV pumping of Tb-based solid-state lasers with visible emission,* The 10th Advanced Lasers and Photon Sources (ALPS2021), online

D. Klimm, T. Hirsch, C. Guguschev, C. Kränkel, *Rare earth oxide systems for substrate and laser applications,* 24. Kalorimetrietage, Braunschweig, online

C. Kränkel, A. Uvarova, L. Hülshoff, C. Guguschev, S. Kalusniak, and D. Klimm, *Czochralski-growth of mixed sesquioxide crystals,* 10th German-French Workshop on Oxide, Dielectric, and Laser Crystals, Idar-Oberstein, Germany,

L. Ladenstein, J. Ring, S. Smetaczek, M. Kubicek, S. Ganschow, G. J. Redhammer, A. D. Knez, G. Kothleitner, I. Dugulan, D. Siegel, A. Limbeck, M. Wilkening, J. Fleig, D. Rettenwander, *Co^{3+}/La^{3+} cross-diffusion at the $Li_7La_3Zr_2O_{12}$ | $LiCoO_2$ interface,* 239th ECS Meeting with the 18th International Meeting on Chemical Sensors (IMCS), Chicago, USA

F. Mauerhoff, S. Püschel, C. Kränkel, and H. Tanaka, *Laser cooling of Yb^{3+}-doped CaF_2 and SrF_2 crystals,* Advanced Solid-State Lasers Conference 2021, online

F. Mauerhoff, S. Püschel, C. Kränkel, and H. Tanaka, *Anti-stokes laser cooling of ytterbium-doped fluorite-structure crystals,* DPG annual meeting, Matter and Cosmos section 2021, online, 2021

W. Miller, R. Schewski, M. Albrecht, S. Bin Anooz, A. Popp, *Kinetic Monte Carlo simulations for homoepitaxy on Ga2O3(100),* 22nd American Conference on Crystal Growth and Epitaxy (ACCGE-22), USA, online

J. Pal, A. Enders-Seidlitz, and K. Dadzis, *Model experiments for heater concepts in Czochralski crystal growth processes,* presented at the 10th International Conference on Electromagnetic Processing of Materials (EPM), Riga, Latvia (online), June 14-16, 2021.

J. Pal, A. Enders-Seidlitz, and K. Dadzis, *Accurate thermal measurements in crystal growth environments,* presented at the Deutsche Kristallzüchtungstagung (DKT), October 6-8, 2021, Berlin, Germany.

S. Püschel, F. Mauerhoff, S. Kalusniak, C. Kränkel, and H. Tanaka, *Laser cooling of ytterbium-doped fluorite structure crystals CaF_2 and SrF_2,* 10th German-French Workshop on Oxide, Dielectric, and Laser Crystals, Idar-Oberstein, Germany

S. Püschel, F. Mauerhoff, S. Kalusniak, C. Kränkel, and H. Tanaka, *Crystal growth and laser cooling of Yb^{3+}-doped CaF_2 and SrF_2,* 51. Deutsche Kristallzüchtungstagung DKT 2021, Berlin, Germany

S. Püschel, S. Kalusniak, C. Kränkel, and H. Tanaka, *Temperature-dependent spectroscopy of Yb:YLF and prospects for laser cooling,* Conference on Lasers and Electro-Optics (CLEO/Europe-EQEC) 2021, Munich, Germany

S. Püschel, S. Kalusniak, C. Kränkel, and H. Tanaka, *Revisiting temperature-dependent spectroscopy of Yb:YLF,* Conference on Lasers and Electro-Optics (CLEO US 2021), San Jose, USA

M. Schröder, *Kristalline Materialien als Grundlage für moderne Technologien,* 4. Symposium Materialtechnik, Clausthal-Zellerfeld, Germany, online

T. Schröder, *Heutige & künftige Hochleistungsmaterialien für die Leistungselektronik,* Berlin Brandenburger Optik-Tag 2021, online and Berlin, Germany, 2021

J. Schwarzkopf, S. Liang, D. Finck, M. W. Neis, D. Mayer, R. Wördenweber, *Application of (K,Na)NbO_3 thin films in surface acoustic wave sensors,* 27th International Workshop on Oxide Electronics, Genua, Italy

A. Suzuki, C. Kränkel, and M. Tokurakawa, *Sub-9 optical-cycle Kerr-lens mode-locked combined gain media laser based on Tm-doped sesquioxide,* Conference on Lasers and Electro-Optics (CLEO/Europe-EQEC) 2021, Munich, Germany

Talks

A. Suzuki, C. Kränkel, and M. Tokurakawa, *Combined gain media 60 fs Kerr-lens mode-locked laser based on Tm:*Lu_2O_3 *and Tm:*Sc_2O_3, Conference on Lasers and Electro-Optics (CLEO2021), online

A. Suzuki, C. Kränkel, and M. Tokurakawa, *Ultrashort pulse generation from Kerr-lens mode-locked Tm-doped sesquioxide lasers at 2.1 µm,* Advanced Solid-State Lasers Conference 2021, online

H. Tanaka, M. Badtke, L. Ollenburg, S. Kalusniak, C. Kränkel, *Generation of Sub-10-ns Pulses from a Passively Q-switched* Pr^{3+}*:*$LiYF_4$ *Laser,* The 10th Advanced Lasers and Photon Sources (ALPS2021), online

H. Tanaka, S. Kalusniak, E. Castellano-Hernández, and C. Kränkel, *UV-pumping and passive Q-switching of visible Tb:*$LiLuF_4$ *lasers,* SPIE Photonics West 2021, online

H. Tanaka, S. Püschel, F. Mauerhoff, S. Kalusniak, and C. Kränkel, *Temperature-dependent radiative lifetime of ytterbium-doped fluoride crystals,* 10th German-French Workshop on Oxide, Dielectric, and Laser Crystals, Idar-Oberstein, Germany

A. Uvarova, S. Kalusniak, C. Guguschev, and C. Kränkel, *OFZ-growth of* $Yb{:}(Sc,Y)_2O_3$ *for 1 µm lasers,* Conference on Lasers and Electro-Optics (CLEO/Europe-EQEC) 2021, Munich, Germany

C. Guguschev, C. Richter, M. Brützam, K. Dadzis, J. Schreuer, C. Hirschle, T.M. Gesing , A. Kwasniewski, and D. G. Schlom, *Revisiting the growth of large (Mg,Zr):SrGa12O19 single crystals: Core formation and its impact on structural homogeneity revealed by correlative X ray imaging*. Deutsche Kristallzüchtungstagung DKT 2021, Berlin, Germany

Patents

Crystal growth in magnetic fields (semiconductors group III–V, IV)

Ch. Frank-Rotsch, P. Rudolph, O. Klein, B. Nacke, R.-P. Lange
Vorrichtung und Verfahren zur Herstellung von Kristallen aus elektrisch leitenden Schmelzen
(Device and method for producing crystals from electrically conductive melts)
DE102007028548B4; EP2162571B1 (08784553.3) (DK, ES, FR, NO) KRIST*MAG*®

R.-P. Lange, D. Jockel, B. Nacke, H. Kasjanow, M. Ziem, P. Rudolph, F. Kießling, Ch. Frank-Rotsch, M. Czupalla
Vorrichtung zur Herstellung von Kristallen aus elektrisch leitenden Schmelzen
(Device for producing crystals from electro-conductive melts)
DE102007028547B4; EP 2162570B1 (08784554.1) (DK, ES, FR, NO) KRIST*MAG*®

Ch. Frank-Rotsch, P. Rudolph, R.-P. Lange, D. Jockel
Vorrichtung und Verfahren zur Herstellung von Kristallen aus elektrisch leitenden Schmelzen
(Device and method for producing crystals from electrically conductive melts)
DE102007046409B4 KRIST*MAG*®

M. Ziem, P. Rudolph, R.-P. Lange
Vorrichtung zum Züchten von Einkristallen aus elektrisch leitfähigen Schmelzen
Device for the manufacture of crystals from electrically conductive melts
DE102007020239B4 KRIST*MAG*®

R.-P. Lange, P. Rudolph, M. Ziem
Vorrichtung zur Herstellung von Kristallen aus elektrisch leitenden Schmelzen
(Device for producing crystals from electro-conductive melts)
DE102008035439B4

F. Büllesfeld, N. Dropka, W. Miller, U. Rehse, U. Sahr, P. Rudolph
Verfahren zum Erstarren einer Nichtmetall-Schmelze
(Method for freezing a nonmetal melt)
EP 2370617B1 (09749132.8) (DE, ES, IT, NO, FR, GB), TW 201035391

N. Dropka, P. Rudolph, U. Rehse
Verfahren zur Herstellung von Kristallblöcken hoher Reinheit
(Method for the preparation of crystalline blocks of high purity)
DE102010028173B4

Patents

N. Dropka, Ch. Frank-Rotsch, P. Lange, M. Ziem
Verfahren und Vorrichtung zur gerichteten Kristallisation von Kristallen aus elektrisch leitenden Schmelzen
(Method and device for the manufacture of crystals by directed solidification from electrically conducting melts)
DE102012204313B3

N. Dropka, Ch. Frank-Rotsch, P. Rudolph, R.-P. Lange, U. Rehse
Kristallisationsanlage und Kristallisationsverfahren zur Herstellung eines Blocks aus einem Material, dessen Schmelze elektrisch leitend ist
(Crystallization system and crystallization process for producing a block from a material with an electrically conductive molten mass)
DE102010041061B4

M. Czupalla, B. Lux, F. Kießling, O. Klein, P. Rudolph, W. Miller, M. Ziem, F. Kirscht, R.-P. Lange
Verfahren zur Züchtung von Kristallen aus elektrisch leitenden Schmelzen, die in der Diamant- oder Zinkblendestruktur kristallisieren
(Method for growing crystals that crystallize in diamond or zinc blende structure from electrically conductive melts)
DE102009027436B4

F. Kießling, , P. Rudolph, Ch. Frank-Rotsch, N. Dropka
Verfahren zur gerichteten Kristallisation von Ingots
(Method for the directed solidification of ingots)
DE102011076860B4

N. Dropka, Ch. Frank-Rotsch, P. Lange, P. Krause
Kristallisationsanlage und Kristallisationsverfahren zur Kristallisation aus elektrisch leitenden Schmelzen sowie über das Verfahren erhältliche Ingots
(Crystallisation system and crystallisation method for crystallisation from electrically conductive melts, and ingots that can be obtained by means of the method)
DE102013211769A1

J. Boschker, Ch. Frank-Rotsch, M. Zorn, T. Schröder
Substrat für ein Halbleiterbauelement Halbleitervorrichtung und Verfahren zum Herstellen eines Substrats für ein Halbleiterbauelement
(Semiconductor device and method for producing a substrate for a semiconductor component, and use of indium during production of same)
DE102020131850, PCT/EP2021/082758

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KRIST*MAG*®

Semiconductors group IV

M. Wünscher, H. Riemann
Vorrichtung für das tiegelfreie Zonenziehen von Kristallstäben

(Apparatus for continuous zone-melting a crystalline rod)
DE102012022965B4, EP 2920342B1 (DE, DK, LV)

N. Abrosimov, J. Fischer, H. Riemann, M. Renner
Verfahren und Vorrichtung zur Herstellung von Einkristallen aus Halbleitermaterial
(Process and apparatus for producing semiconductor single crystals)
EP2504470B1 (NO, ES, NL, FR, DK, GB, BE, IT), DE102010052522B4, JP 5484589B2, US 9422636

Oxides

Z. Galazka, R. Uecker, D. Klimm, M. Bickermann
Method for growing beta phase of gallium oxide (ß-Ga2O3) single crystals from the melt contained within a metal crucible
EP3242965B1 (AT, BE, CH, DE, CZ, ES, FR, GB, IT, NL, PL), KR101979130B1, US11028501B2, JP7046117B2

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
EP2841630B1 (DE, BE, FR, GB, IT), US10208399B2, JP6134379B2

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
Verfahren und Vorrichtung zum Züchten eines Seltenerd-Sesquioxid-Kristalls
(Method and apparatus for growing a rare earth sesquioxide crystal)
DE102020120715, PCT/EP2021/068687

S. Ganschow, Ch. Kränkel
Oxidkristall mit Perowskit-Struktur
(Oxide crystal with perovskite structure)
DE 102021134215.5

Patents

Aluminium nitride

A. Dittmar, C. Hartmann, J. Wollweber, M. Bickermann
(Sc, Y):AlN Einkristalle für Gitter-angepasste AlGaN Systeme
((Sc,Y):AlN single crystals for lattice-matched AlGaN systems)
DE102015116068A1, KR1020180048926A

Semiconducting Layers/Nanostructures

T. Boeck, R. Heimburger, G. Schadow, H.-P. Schramm, J. Schmidtbauer, T. Teubner, R. Fornari
Kristallisationsverfahren zur Erzeugung kristalliner Halbleiterschichten
(Crystallization method for producing crystalline semiconducting layers)
DE102010044014A1

O. Ernst, T. Boeck, F. Lange, H.-P. Schramm, T. Teubner, D. Uebel
Verfahren zur Mikrostrukturierung
(Method for microstructuring)
DE102020126553, PCT/EP2021/076794

D. Uebel, R. Bansen, T. Boeck, O. Ernst, H.-P. Schramm, T. Teubner
Silizium-basierte Wafer und Verfahren zur Herstellung von Silizium-basierten Wafern
(Silicon-based wafers and method of manufacturing silicon-based wafers)
DE102020132900, PCT/EP2021/083974

Oxide Layers

M. Albrecht, A. Baki, K. Irmscher, T. Schulz, J. Schwarzkopf, J. Stöver
Verfahren zum Herstellen eines Kristalls mit Perowskitstruktur
(Formingless Resistive Switching by Off-Stoichiometry Control of ABO3 Perovskites)
DE1020132049

T. Chou, A. Popp, W. Häckl
Method for producing a gallium oxid layer on a substrate
EP 21187231.2

Characterization

P. Gaal
Bereitstellen eines transienten Gitter
(Providing a transient grid)
DE102019132393B4, PCT/EP2020/082942

Teaching and Education

Matthias Bickermann
Kristallzüchtung I: Grundlagen und Methoden / Crystal Growth I: Fundamentals and methods
Kristallzüchtung II: Methoden und Anwendungen / Crystal Growth II: Methods and applications
Technische Universität Berlin, Institute of Chemistry

Detlef Klimm
Phasendiagramme / Phase Diagrams
Humboldt-Universität zu Berlin, Department of Chemistry

Christian Kränkel, Tim Schröder (HU Berlin)
Applied Photonics
Humboldt-Universität zu Berlin, Department of Physics

Martin Schmidbauer
Röntgenstreuung: Grundlagen und Anwendung in der Materialwissenschaft / X-Ray Scattering: Basics and Applications in Materials Science
Humboldt-Universität zu Berlin, Department of Physics

Thomas Schröder, Jens Martin, Ted Masselink (HU Berlin)
New directions in electronics, optoelectronics, and devices
Humboldt-Universität zu Berlin, Department of Physics

Thomas Schröder, Radhakrishnan Sumathi, Jens Martin
Grundlagen und Methoden der modernen Kristallzüchtung / Fundamentals and methods of modern crystal growth
Humboldt-Universität zu Berlin, Department of Physics

P. Gaal
Physik für Nanowissenschaftler A
Universität Hamburg, Institut für Nanostruktur und Festkörperphysik
Proseminar: Grundlagen Nanostrukturierter Festkörper
Universität Hamburg

Membership in Committees

Committees

M. Bickermann

- IGAFA e.V. - the scientific network of the non-university research institutions located in Berlin-Adlershof e.V.; member of the board
- DFG Review Board 406-03: Thermodynamics and Kinetics as well as Properties of Phases and Microstructure of Materials; elected member
- Forschungsverbund Berlin: Marthe-Vogt price; member oft he awarding committee

D. Klimm

- Commission on Crystal Growth and Characterization of Materials der International Union of Crystallography (IUCr); consultant
- Deutsche Gesellschaft für Kristallographie (DGK), member of the scientific college (German Society for Crystallography (DGK); member of the Wissenschaftskolleg

T. Schröder

- DESY Photon Science Committee; member
- Forschungsverbund Berlin e.V.;
  executive committee spokesman (from September 2021, deputy spokesman until August 2023)
- Forschungsverbund Berlin e.V.; member nomination committee for the Managing Director
- Humboldt Universität zu Berlin: Strategic committee of the Department of Physics; member
- Leibniz Association: Leibniz Mentoring Program; member
- Leibniz Association: Strategy Forum on Technological Souvereignty; speaker

C. Frank-Rotsch

- Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung (DGKK) (German Association for Crystal Growth); secretary
- European Network of Crystal Growth ENGC; member of the council
- International Organization for Crystal Growth IOCG; member of the executive committee

Conference Committees

C. Guguschev

- Commission on Crystal Growth and Characterization
- of Materials of the International Union of Crystallography
- (IUCr); consultant

P. Gaal

- Beamtime Allocation Panel C09
- European Synchrotrons ESRF

M. Bickermann

- Deutsche Kristallzüchtertagung DKT 2021 (annual meeting of the German Association of Crystal Growth), Berlin, Germany; chair
- Advanced Solid State Lasers Conference ASSL 2021, online; member of the program committee
- 7th European Conference on Crystal Growth (ECCG7), Paris, France; member of the program committee
- International Workshop on Crystal Growth and Technology (IWCGT-8), Berlin, Germany; chair
- 14th International Conference on Nitride Semiconductors (ICNS-14), Fukuoka, Japan; member of the program committee
- 19th International Conference on Defects-Recognition, Imaging and Physics in Semiconductors (DRIP19), online; member of the steering committee
- 5th International Workshop on UV Materials and Devices (IWUMD), Jeju Island, Korea; member of the program committee

N. Dropka

- IKZ-WIAS virtual workshop; co-organizator and chair
- IKZ-BTU-LZKI virtual workshop on artificial intelligence; co-organizator

C. Frank-Rotsch

- International Conference on Crystal Growth and Epitaxy ICCGE-20, Naples, Italy; member of the international advisory board
- 7th European Conference on Crystal Growth (ECCG7), Paris, France; member of the program committee
- Deutsche Kristallzüchtertagung DKT 2021 (annual meeting of the German Association of Crystal Growth), Berlin, Germany; member of the organization team

F. M. Kießling

- International Workshop on Crystal Growth and Technology (IWCGT-8), Berlin, Germany; member of the steering committee

C. Kränkel

- SPIE Photonics West, Solid State Lasers XXX: Technology and Devices, San Francisco, USA; member of the program committee

W. Miller

- International Conference on Crystal Growth and Epitaxy-ICCGE-20, Naples, Italy; member of the international advisory board
- 7th European Conference on Crystal Growth (ECCG7), Paris, France; member of the international scientific committee
- Deutsche Kristallzüchtertagung DKT 2021 (annual meeting of the German Association of Crystal Growth), Berlin, Germany; member of the organization team

J. Schwarzkopf
- DPG annual meeting, focus session: *Functional metal oxides for novel applications and devices*, online; co-organizator

R. Radhakrishnan Sumathi
- International Worskhop on Crystal Growth and Technology (IWCGT-8), Berlin, Germany; co-chair
- Deutsche Kristallzüchtertagung DKT 2021 (annual meeting of the German Association of Crystal Growth), Berlin, Germany; member of the organization team
- International Conference on Recent Trends in Applied Science and Technology ICRTAST, Trichy, India; member of the scientific advisory committee

Editorial board membership

M. Bickermann
- Progress in Crystal Growth and Characterization of Materials, Elsevier, associate editor
- Journal of Crystal Growth; editor

N. Dropka
- Crystals, topic editor; guest editor for special issue "Artificial intelligence for crystal growth and characterization"

C. Kränkel
- Optics Express, associate editor

W. Miller
- Crystals, member of editorial board

Guest Scientists

Prof. Darrell Schlom
Cornell University, USA
18.10.2021 – 22.10.2021

Dr. Hamada Maki
Kanazawa University, Japan
07.10.2020 - 31.10.2021

Yankun Wang
Xi'an Jiaotong University, China
11.03.2021 – 31.03.2023

Dr. Anna Suzuki
The University of Electro-Communications, Tokyo, Japan
11.10.2021 – 31.10.2022

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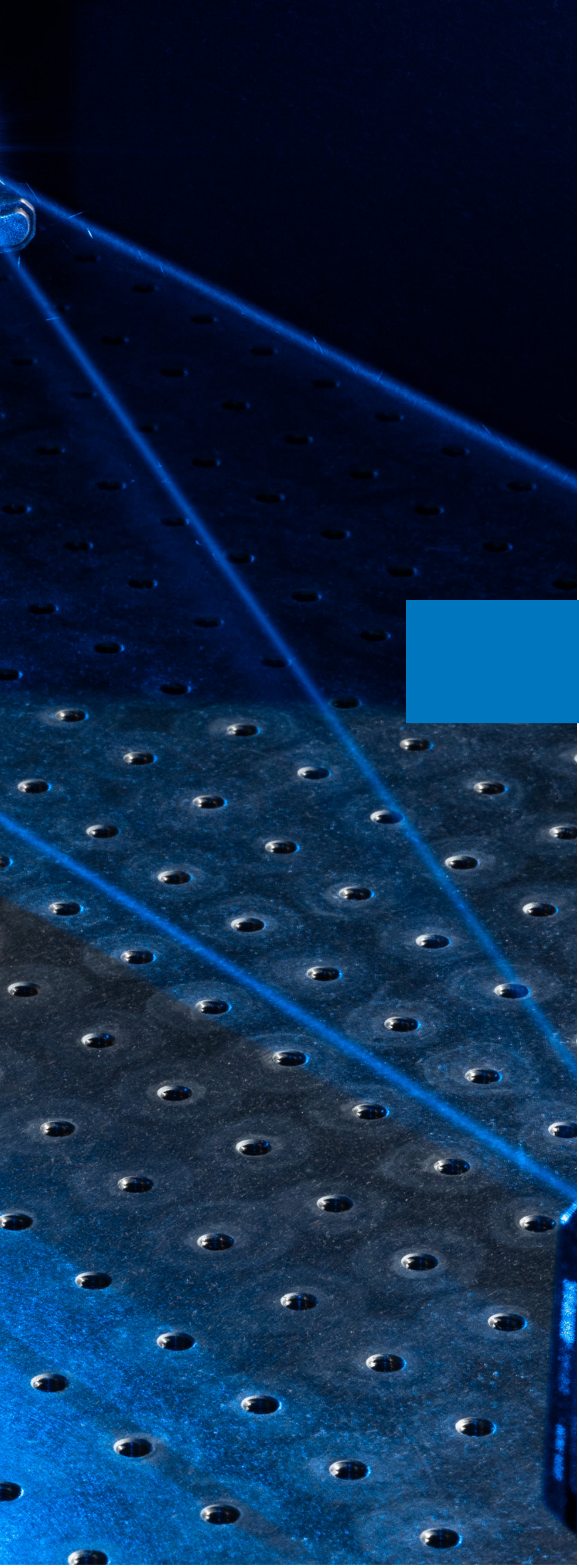

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