Annual Report

Leibniz-Institut für Kristallzüchtung

im Forschungsverbund Berlin e.V.

2020

ikz

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2020

Preface

Sehr geehrte Leserinnen und Leser,

*das Jahr 2020 zwang uns in vielerlei Hinsicht aufgrund der Covid-19 Pandemie neue Wege in der Organisation unserer Arbeitsabläufe zu gehen. Sicher führten diese Einschränkungen im Alltag, miteinander nur vereinzelt und auf Distanz arbeiten zu können, unweigerlich zu einem Effizienzverlust für ein stark experimentell arbeitendes Institut wie das unserige. Dennoch fanden wir stets Mittel und Wege, unsere Ziele auch weiterhin erfolgreich zu verfolgen. Herausgehoben seien hier unsere Bemühungen im Bereich der Digitalisierung. Durch die Ausgabe von Laptops an die IKZ Kolleg*innen, den Ausbau des WLAN Systems und den Aufbau professioneller Videokonferenz-Systeme im Hause schafften wir mit großem finanziellem Engagement eine professionelle Hardware-Basis, um Informationen für die wissenschaftliche, technologische und administrative Arbeit stets zeitnah fließen zu lassen. Die Einführung des elektronischen Bestellsystems, des elektronischen Zeitmanagementsystems sowie der elektronischen Personalakte bildeten die Basis für den effizienten Ablauf der Verwaltungsvorgänge – insbesondere in enger Wechselwirkung mit den Kolleg*innen der Gemeinsamen Verwaltung des Forschungsverbundes e.V. Mit entsprechenden IT Betriebsvereinbarungen und IT Nutzerordnungen hinterlegten wir ferner in transparenter Weise eine Governance-Struktur, wie wir hier miteinander im Hause arbeiten möchten.*
Unsere Öffentlichkeitsarbeit war in diesem Jahr besonders gefordert, um die Kommunikation aufrecht zu erhalten. Der monatlich erscheinende IKZ Newsletter etablierte sich dabei als wichtiges Informationsmedium für allgemeine Institutsinformationen.

Wissenschaftlich und technologisch finden Sie in diesem IKZ Jahresbericht 2020 wieder eine Vielzahl spannender News, Highlights & Forschungsberichte. Herausheben möchte ich in diesem Jahr dabei die Entwicklungen um die Floatzone (FZ) Silizium (Si)-Züchtung im Hause mit einer Gesamtinvestition von zirka 2,5 Millionen €. Nach langjähriger Entwicklung gemeinsam mit der Firma PVATepla wurde die FZ30 Anlage mit dem Potential für die 8" FZ-Si Kristallzüchtung im Hause unter erschwerten Covid-Bedingungen in 2020 installiert und bereits erfolgreich in Betrieb genommen. Neben der FZ-Züchtungsanlage mussten wir für diese Kristallgröße auch die umgebende Infrastruktur wie Ätzlabore usw. substanziell ertüchtigen. An spannenden Aufgaben gibt es keinen Mangel: Das IKZ ist nun wieder anschlussfähig an den 'state-of-the-art' der Industrie im Bereich des FZ-Si Materials für die in der Energiewende boomende Leistungselektronik. Darüberhinaus wird FZ-Si Material höchster Güte aber auch in anderen Anwendungsgebieten wie der aufkommenden Quantumtechnologie und dem geplanten Einsteinteleskop zur Gravitationswellendetektion dringend benötigt.
Einen grossen Schritt konnten wir im Jahre 2020 im Bereich der Vernetzung und Internationalisierung gehen mit der Gründung von drei Joint Labs mit strategischen Partnern. In Deutschland eröffneten wir mit DESY Hamburg ein Joint Lab im Bereich der modernen Synchrotron- und Freien Elektronenlaserforschung, mit unseren langjährigen Partnern in Cornell in den USA im Bereich der Oxidelektronik und mit der Jiaotong Universität in Xi´an in China im Bereich der dielektrischen Filme. Diese Zusammenarbeit wird uns neben Lehre und Forschung auch strategische Einblicke in F & E Trends und aufkommende Themen frühzeitig geben.

Eine große Freude ist mir die Eröffnung des neuen IKZ Eingangsbereiches nach mehrjähriger Planungs- und Bauzeit im Oktober 2020. Mit dieser Modernisierung des Foyers schaffen wir uns eine attraktive Fläche im Hause für Begegnungen miteinander in unseren Arbeitspausen sowie zum Empfang von Gästen und Besuchern. Dieser Begrüßungsbereich wird auch eine kleine Ausstellung beherbergen, die vor dem Besuch des Institutes erste Einblicke in die Bedeutung unserer Forschungs- und Entwicklungsarbeiten für die Gesellschaft gibt. Ein Catering bei größeren Veranstaltungen im Hause wird hier künftig ebenfalls möglich sein und eine neue Terrasse vor dem Foyer mit weiteren Abstellmöglichkeiten für Fahrräder soll der sich wandelnden Mobilität in Berlin Rechnung tragen.

Besuchen Sie uns gerne am Institut! Bis dahin wünschen wir Ihnen eine informative und unterhaltsame Lektüre des IKZ-Jahresberichts 2020.

Mit freundlichen Grüßen

Thomas Schröder

Preface

Dear Readers,

2020 was in many ways a year that forced us to find new ways of organising our workflows due to the Covid-19 pandemic. As an institute with a highly experimental approach like ours, these restrictions in our daily routines, such as working with each other only from a distance and in isolation, unavoidably led to a loss of efficiency. Nevertheless, we were always able to find ways and means to remain successful in pursuing our goals. Special emphasis should be placed here on our efforts in the area of digitisation. By providing laptops to the staff of the IKZ, extending the Wi-Fi system and setting up professional video-conferencing systems, we created a professional hardware basis with great financial commitment enabling information for scientific, technological and administrative work to flow in a timely manner. The introduction of the electronic ordering system, the electronic time management system as well as the electronic personnel file provided the basis for the efficient flow of administrative processes, especially in close interaction with the colleagues of the Joint Administration of Forschungsverbund e.V. Moreover, we established a governance structure in a transparent manner by means of corresponding IT works agreements and IT user regulations to define how we would like to work with each other here at the Institute. Our public relations work was especially demanding this year as we had to maintain communication. In this context, the monthly IKZ newsletter became an important medium for sharing general information about the Institute.

This IKZ Annual Report 2020 once again presents a multitude of fascinating scientific and technological news, highlights and research reports. This year, I would like to draw your attention to the developments around the float zone (FZ) silicon (Si) growth in our Institute with a total investment of about €2.5 million. In 2020, after many years of development together with PVATepla, the FZ30 system with the potential for 8″ FZ-Si crystal growth was installed in-house under difficult Covid conditions and has already been successfully put into operation. Apart from the FZ growth system, we also had to substantially enhance the surrounding infrastructure such as etching laboratories etc. for this crystal size. There is no lack of exciting tasks: Now, the IKZ is again able to compete with the 'state-of-the-art' of the industry in the field of FZ-Si material for power electronic systems, which is booming in the wake of the energy turnaround. Furthermore, there is an urgent need for FZ-Si material of the highest quality also in other application areas such as the emerging quantum technology and the planned Einstein telescope for gravitational wave detection.

Another major step was taken in 2020 in networking and internationalization when we set up three joint labs with strategic partners. With DESY Hamburg in Germany, we opened a Joint Lab in the field of modern synchrotron and free electron laser research, together with our long-term partners in Cornell, USA, in the field of oxide electronics and with Jiaotong University in Xi'an, China, in the field of dielectric films. Apart from teaching and research, this cooperation will also give us strategic insights into R & D trends and upcoming topics at an early stage.

The opening of the new IKZ entrance area in October 2020 after several years of planning and construction work fills me with great joy. With this modernisation of the foyer, we have created an attractive area in the building as a meeting point during our work breaks and for welcoming guests and visitors. This reception area will also feature a small exhibition offering first insights into the importance of our research and development work for the society before visiting the Institute. Here, it will also be possible in the future to provide catering for larger in-house events, and a new terrace in front of the foyer with additional bicycle parking facilities will meet the needs of Berlin's changing mobility.

You are welcome to visit us at the Institute! In the meantime, we hope you find the IKZ Annual Report 2020 informative & entertaining.

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

The Institute

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

The Institute

- 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 Schlüssel-technologien
- 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

- 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

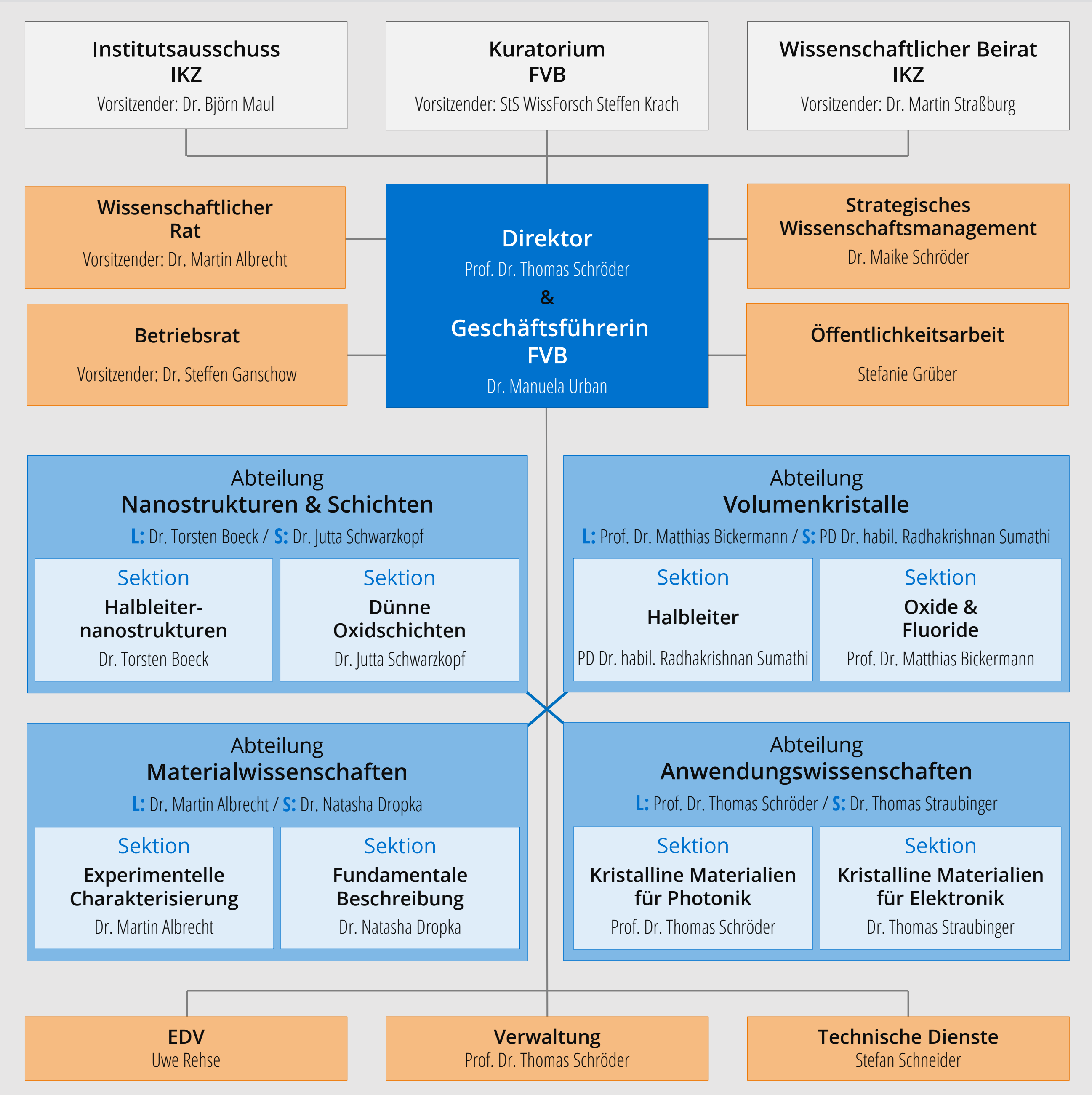
IKZ as family-friendly employer

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 2020
Organisation Chart 2020



Wissenschaftlicher Beirat 2020
Scientific Advisory Board 2020

Dr. Martin Strassburg (chair)
Osram Opto Semiconductors GmbH,
Regensburg, Germany

Prof. Dr. Saskia Fischer (vice chair)
Department of Physics,
Humboldt-Universität zu Berlin, Germany

Prof. Dr. Anna Fontcuberta I Morral
Laboratory of Semiconductor Materials,
Ecole Polytechnique Fédérale de Lausanne,
Switzerland

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

Prof. Dr. Lena F. Kourkoutis
School of Applied and Engineering Physics,
Cornell University, NY, USA

Dr. Georg Schwalb
Siltronic AG,
Burghausen, Germany

Prof. Dr. Thomas Südmeyer
Université de Neuchâtel,
Institute for Physics,
Neuchâtel, Switzerland

Prof. Dr. Götz Seibold
Brandenburgische Technische Universität
Cottbus-Senftenberg,
Cottbus, Germany

Prof. Dr. Bernd Tillack
Leibniz-Institut für innovative Mikroelektronik,
Frankfurt/Oder, Germany

Vertreter des Landes Berlin
Representative of the State of Berlin

Dr. Björn Maul
Senatskanzlei – Wissenschaft und Forschung,
Berlin

Vertreter der Bundesrepublik Deutschland
Representative of the Federal Republic of Germany

Ingo Hoellein
Bundesministerium für Bildung und Forschung,
BMBF Bonn / Berlin

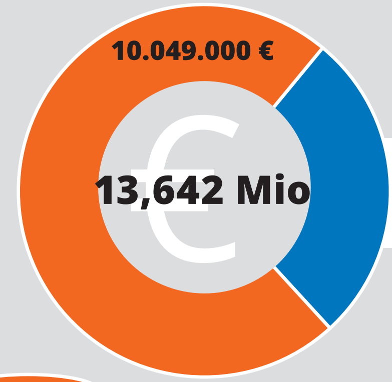
The Institute

2020 in Zahlen
2020 in figures

Budget

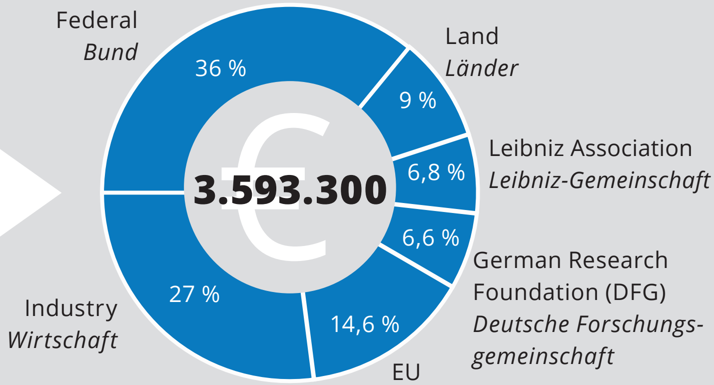
Gesamt
Total

Institutional funding
Institutionelle Förderung

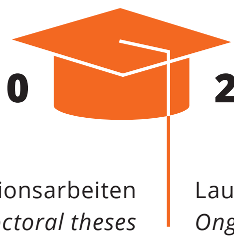


3.593,300 €
Third-party funding
Drittmittelförderung

Drittmittelförderung
Third-party funding



Lehre
Education



0
Abgeschlossene Promotionsarbeiten
Defended doctoral theses

20
Laufende Promotionsvorhaben
Ongoing dissertations

Publikationen
Publications

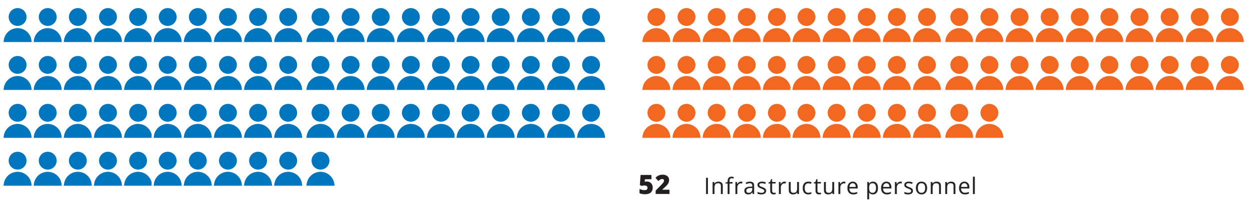
Artikel in referierten (peer-review) Journalen
Articles in peer-reviewed journals

Kapitel in Büchern
Chapters in books

Stichtag 31.12.2020

Personal gesamt
Staff total*

123

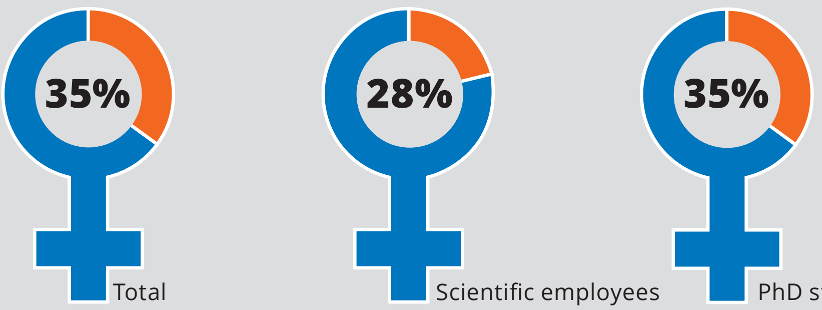


52 Infrastructure personnel
Infrastrukturpersonal

71 Scientific employees
Wissenschaftliche Mitarbeiter/innen

* not including Bachelor-/Master students and student assistants.
ohne Bachelor-/Masterstudenten und studentische Hilfskräfte.

Frauenanteil
Female proportion

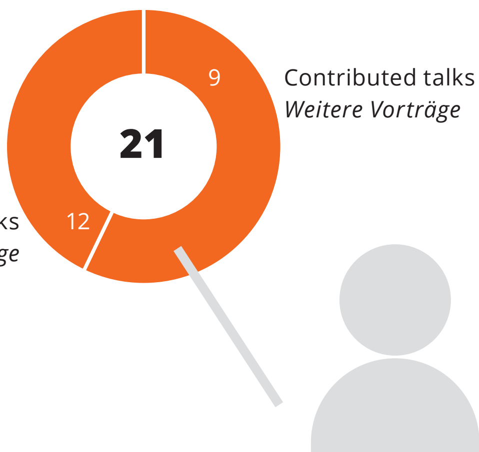


Total
Gesamt

Scientific employees
Wissenschaftliche Mitarbeiterinnen

PhD students
Doktorandinnen

Beiträge auf internationalen Konferenzen
Contributions in international conferences



Contributed talks
Weitere Vorträge

Invited talks
Eingeladene Vorträge

Gleichstellung in der Leibniz-Gemeinschaft, im Forschungsverbund Berlin und am IKZ:

Ein zentrales Ziel des Paktes für Forschung & Innovation IV (2021–2030)

Ein Interview mit Prof. Dr. Heribert Hofer (Gleichstellungsbeauftragter des Forschungsverbundes Berlin (FVB) e.V.), Marta Alirangues (Zentrale Gleichstellungsbeauftragte des FVB), Prof. Dr. Thomas Schröder (Wissenschaftlicher Direktor des IKZ) sowie Iryna Buchovska & Lisa Picard (Gleichstellungsbeauftragte des IKZ).
Gleichstellung zu befördern ist eine zentrale und stete Aufgabe in der Leibniz-Gemeinschaft. Unsere Gemeinschaft hat sich hierzu im Pakt IV für Forschung & Innovation (2021-2030) zur Zielerfüllung verpflichtet. Im Jahre 2020 erschien der Bericht zur Umsetzung der Leibniz-Gleichstellungsstandards in den Einrichtungen der Leibniz-Gemeinschaft. Ebenso wurde zum ersten Mal in der Geschichte des FVB e.V. eine zentrale Gleichstellungsbeauftragte ins Amt gewählt. Was bedeutet dies für die anstehenden Aufgaben im FVB e.V. und die beteiligten Institute? Anhand der fünf Grundsätze des Leibniz-Gleichstellungsstandards diskutierten die FVB Kolleg*innen die aktuelle Situation im FVB e.V. und am IKZ.

Thomas Schröder:
„Der Leibniz-Bericht zur Umsetzung der Gleichstellungsstandards zeigt die spezifischen Verdienste, aber auch die Herausforderungen in den Einrichtungen der Leibniz-Gemeinschaft auf, um unseren Präsidenten Herr Matthias Kleiner zu zitieren. Die Frage ist somit für uns, an welchen Stellen wir besser werden können. Hierzu würde ich mich gern an den 5 Grundsätzen der Leibniz-Gleichstellungsstandards orientieren. Der Grundsatz 1 zielt auf ***Frauen in Leitungspositionen*** *ab. Was denken Sie, welche Möglichkeiten wir hier haben?“*

Heribert Hofer:
„Uns stehen in diesem Bereich eigentlich 4 Tools zur Verfügung, die von verschiedenen Instituten gelebt werden: Offene Ausschreibungen, geteilte Führung, Teilzeit sowie Nachwuchsgruppen. Gerade die offenen Ausschreibungen sind ein großer Vorteil für Frauen. Wenn Positionen nicht durch aktive Rekrutierung intern besetzt werden, sondern ausgeschrieben werden, hat jede die Möglichkeit davon Kenntnis zu nehmen. Im besten Fall folgt der Ausschreibung noch eine externe aktive Rekrutierung. Das steigert die Chancen von Frauen immens.“

Gender equality at the Leibniz Association, the Forschungsverbund Berlin and the IKZ:

A central goal of the Joint Initiative for Research & Innovation IV (2021–2030)

An interview with Prof. Dr. Heribert Hofer (Equal Opportunities Officer of the Forschungsverbund Berlin (FVB) e.V.), Marta Alirangues (FVB Central Equal Opportunities Officer), Prof. Dr. Thomas Schröder (Scientific Director of the IKZ) and Iryna Buchovska & Lisa Picard (Equal Opportunities Officer of the IKZ).
It is a central and constant task of the Leibniz Association to promote gender equality. To achieve this goal, our Association has committed itself in the Joint Initiative IV for Research & Innovation (2021-2030). In 2020, the Report on the Implementation of the Leibniz Equality Standards at the Institutes of the Association was published. In addition, a Central Equal Opportunity Officer was elected into office for the first time in the history of the FVB e.V. What does this mean for the forthcoming tasks in the FVB e.V. and the participating Institutes? The FVB colleagues discussed the current situation at the FVB e.V. and the IKZ with regard to the 5 Principles of the Leibniz Equality Standard.

Thomas Schröder:
"The Leibniz Report on the Implementation of the Equality Standards highlights the specific accomplishments but also the challenges in the Institutes of the Leibniz Association, to quote our President Mr. Matthias Kleiner. Therefore, the question for us is at which points we can make improvements. I would like to base this on the 5 Principles of the Leibniz Equality Standards. Principle 1 refers to ***women in leadership positions****. What opportunities do you think we have here?"*

Heribert Hofer:
"In this field, we actually have 4 tools at our disposal, which are applied and used by different Institutes: open job postings, shared leadership, part-time as well as junior research groups. Especially the open job postings are a big advantage for women. If vacant positions are not filled internally through active recruitment, but are openly advertised, everyone has the opportunity to take note of it. Ideally, the open job posting is followed-up by external active recruitment. This increases the chances of women immensely."

The Institute

Thomas Schröder:
*„Ja, da stimme ich voll zu. Am IKZ haben wir das sehr positiv gelebt. Bezüglich der offenen Ausschreibungen haben wir gerade eine Betriebsvereinbarung „Stellenausschreibungen" verabschiedet. Wichtig in diesem Bereich ist auch, dass die Gleichstellungsbeauftragten hier frühzeitig mit auf den Ausschreibungstext schauen können. Besonders wichtig wäre dies bei der Ausschreibung von Direktor*inpositionen."*

Marta Alirangues:
„Ja, es ist in diesem Bereich sehr wichtig, darauf zu achten, dass der Anzeigentext möglichst unvoreingenommen ist, vor allem, wenn es ein Ungleichgewicht zwischen den Geschlechtern bei der Besetzung von Stellen gibt. In Stellenanzeigen werden oft Worte verwendet, die in unserer Gesellschaft üblicherweise Männern zugeschrieben werden. Außerdem gibt es einen großen Unterschied zwischen Frauen und Männern, wenn sie sich auf eine Stelle bewerben: Während Frauen an sich selbst die Ansprüche stellen, alle in der Stellenbeschreibung aufgeführten Anforderungen zu erfüllen, sehen Männer das eher lockerer und bewerben sich auch dann, wenn einige Aspekte nicht auf sie zutreffen. Es ist wichtig zu verstehen, welche Formulierungen Frauen ansprechen und wie man die Ausschreibung gestaltet. Es gibt nützliche Tools, die dabei helfen, die Richtung der Voreingenommenheit im Anzeigentext zu erkennen, sowohl auf Englisch als auch auf Deutsch:

- English: **http://gender-decoder.katmatfield.com/**
- Deutsch: **https://genderdecoder.wi.tum.de/**

Thomas Schröder:
„Wir haben am IKZ außerdem die Erfahrung gemacht, dass eine geteilte Führung / Doppelspitze in den einzelnen Abteilungen ein weiteres gutes Instrument ist, um Führungspositionen für Frauen attraktiver zu gestalten. Das Modell erlaubt die Teilung administrativer Belastungen und wurde gut angenommen. Auf der anderen Seite muss man leider sagen, dass es uns nicht gelungen ist, unsere Nachwuchsgruppen paritätisch zu besetzen. Da diese Positionen die nächste Generation an Führungspersönlichkeiten vorbereiten, tragen wir hier dazu bei, dass sich weiterhin ein ´Bottleneck` an Bewerberinnen bildet, was wir verhindern sollten und wollten. Gibt es weitere Erfahrungen im Bereich geteilter Führung oder gar Teil-Zeit-Führung?"

Marta Alirangues:
„Das Problem, auch in unserer heutigen Zeit ist, dass Frauen in der Regel mehr als eine Funktion erfüllen. Neben dem Job kümmern sie sich um die Familie und viele von ihnen engagieren sich für Gleichstellungsfragen und für die Erhöhung der Sichtbarkeit von Frauen in der Wissenschaft. Wenn Frauen also in ihrem Leben an den Punkt kommen, eine Führungsposition einzunehmen, dann haben sie das „Päckchen Familie" meist schon auf dem Rücken und müssen schauen, wie sie das schultern können.

Thomas Schröder:
"Yes, I fully agree. At the IKZ, we have been practising this very successfully. With regard to open postings, we have just passed a Works Agreement "Job Postings". It is also important that the Equal Opportunity Officers can take a look at the text of the advertisement at an early stage. This would be of particular importance when director positions are posted."

Marta Alirangues:
"Yes, it is very *important here to ensure that the text of the job posting is as unbiased as possible, especially in cases where an imbalance exists between the genders when filling vacant positions. In job postings, words are often used that are usually attributed to men in our society. Furthermore, there is a big difference between women and men when they apply for a job: While women place demands on themselves to fulfil all the requirements specified in the job description, men have the tendency to take this more light-heartedly and apply even if some aspects do not really fit the bill. It is important to understand which formulations appeal to women and how the job posting should be prepared. There are useful tools which may help to identify bias tendencies in the job posting text, both in English and in German:*

- English: **http://gender-decoder.katmatfield.com/**
- German: **https://genderdecoder.wi.tum.de/**

Thomas Schröder:
"Moreover, experience at the IKZ has shown that shared management / dual leadership in the individual departments is another good instrument to make management positions more attractive for women. The concept allows the sharing of administrative burdens and has been well accepted. However, we have to admit that we have not succeeded in filling our junior research groups with equal numbers of women and men. As these positions prepare the next generation of leaders, we continue to contribute to a 'bottleneck' of female applicants here, which is something we ought to and wanted to prevent. Are there other experiences in the area of shared management or even part-time management?"

Marta Alirangues:
"Even today, the problem is that women usually have more than one function to fulfil. In addition to the job, they take care of the family and many of them are committed to promoting gender equality and increasing the visibility of women in science. When women finally reach the point in their lives where they want to take on a leadership position, most of them already have the "family package" on their backs and need to figure out how they can shoulder it.

The Institute

Hinzu kommt das Lohngefälle, der Kampf, sich in einer überwiegend von Männern dominierten Welt durchzusetzen und viele andere Probleme, die ihren Zugang zu Führungspositionen erschweren. Eine geteilte Führung kommt ihnen dabei natürlich sehr zugute und sie trauen es sich eher zu. Ich finde das einen wunderbaren Ansatz"

Thomas Schröder:
„Der zweite Grundsatz ist die ***Gleichstellung als Leitprinzip.*** *Interessant ist zum Beispiel, dass im Gleichstellungsbericht zu lesen ist, dass die Anzahl an weiblichen Hauptantragstellern im Leibniz-SAW-Verfahren zurückgeht. Sicherlich liegt das an dem höheren Männeranteil unter den führenden Wissenschaftler*innen. Es stellt sich daher natürlich die Frage, ob wir in diesem Bereich genug tun?"*

Heribert Hofer:
„Bereits im Stellenplan muss das Personalkonzept bezüglich Gleichstellung berücksichtigt werden. Frauen müssen mehr ermutigt werden, entsprechende Positionen zu besetzen. Es steht außer Frage, dass es keine unterschiedliche Bezahlung zwischen den Geschlechtern geben darf sowie eine Förderung von weiblichen Hauptantragstellern im Leibniz-SAW-Verfahren angestrebt werden muss. Eine Möglichkeit wäre, beim internen Ausscheidungsverfahren innerhalb jedes Instituts die Regel zu etablieren, dass bei zwei gleichwertigen Projektideen das Projekt den Zuschlag bekommt, bei dem die Principal Investigators Frauen sind. Ich kenne eine Einrichtung im FVB, die das lebt und die Regel einmal nutzte – das Projekt wurde prompt bewilligt."

Thomas Schröder:
„Absolut! Für mich *könnten wir hier im FVB gemeinsam voranschreiten. Mittels eines Personalkonzeptes, heruntergebrochen für die einzelnen Institute,* können wir *eine Aussage darüber treffen, wo die einzelnen Institute hier stehen. Und wir uns gemeinsam Gedanken machen, zum Beispiel mittels einer Findungskommission, wie die Dinge besser umgesetzt werden könnten. Als baldiger FVB Sprecher werde ich die Gleichstellung hier noch mehr in den Fokus rücken."*
„Kommen wir zum Grundsatz 3: ***Gleichstellungsbeauftragte.*** *Ich bin sehr dankbar dafür, dass wir nun eine zentrale Gleichstellungsbeauftragte für den Forschungsverbund haben. Welche Aufgaben sind mit dieser Position verbunden, Herr Hofer?"*

Heribert Hofer:
„Gleichstellung hat in meinen Augen drei Funktionen: „Controlling", Beratung, Vertretung aller Frauen im FVB. Ich denke, dass die beratende Funktion, wie etwas besser gemacht werden könnte, die wichtigste dabei ist. Daher hätte ich auch einen Verbesserungsvorschlag: Die Belegung der Stelle sollte nicht nur 3 Jahre (eine Periode) lang sein, sondern eher 2 Perioden, eben weil man sehr viel Einarbeitung in dieser Position hat, um in der beratenden Funktion wirklich professionell agieren zu können."

On top of that, there is the wage gap, the struggle to establish themselves in a mainly male-dominated world, and various other problems that make it difficult for them to access leadership positions. The concept of shared leadership naturally benefits women and encourages them to take on such a position. I think that's a wonderful approach."

Thomas Schröder:
"The 2nd Principle is ***equality as a guiding principle****. Interestingly, the Equality Report states that the number of female principal applicants in the Leibniz SAW procedure (SAW - Senate Competition Committee) is waning. This can certainly be attributed to the higher proportion of men among the leading scientists. This naturally raises the question of whether we have been doing enough in this area."*

Heribert Hofer:
"The personnel concept regarding gender equality must already be considered in the employment plan. Women must be more encouraged to take on relevant positions. It goes without saying that there should not be any differences in payment between genders and that female principal applicants in the Leibniz-SAW procedure need to be supported. One option would be to set up the rule in the internal selection procedure within each Institute that if there are two equivalent project ideas, the project in which the principal investigators are women will be awarded the contract. I know an institution in the FVB that did just that and used this rule one time - the project was indeed approved."

Thomas Schröder:
"Absolutely! As far as I am concerned, we could jointly move forward here in the FVB. By means of a personnel concept, broken down to the individual Institutes, we are able to assess how far the individual institutions have already progressed. And together, for example by means of a "Findings Committee", we can think about how things could be implemented more effectively. As the soon-to-be FVB Spokesperson, I am going to put gender equality even more in the spotlight here."
"Now let us move on to Principle 3: ***Equal Opportunity Officers****. I really appreciate that we now have a Central Equal Opportunity Officer for the Forschungsverbund. Which tasks are associated with this position, Mr. Hofer?"*

Heribert Hofer:
"To my mind, gender equality has three functions: "Controlling", consultation, representation of all women in the FVB. I believe the consulting function, showing how something could be changed for the better, is the most important function. Therefore, I have a suggestion for improvement: the position should not only be held for 3 years (1 period), but rather for 2 periods, simply because you need a lot of induction and orientation in this position, in order to act in the consulting function in a truly professional way."

The Institute

Thomas Schröder:
*„Lieber Heribert, danke fuer diese schöne Zusammenfassung. Frau Aliranguez wird uns regelmäßig im FVB Vorstand über ihre Arbeit & Empfehlungen berichten; die Direktor*innen müssen sie entsprechend unterstützen. Lasst mich zum nächsten Grundsatz 4 fortfahren, der die* ***Vereinbarkeit von Beruf und Familie*** *im Blick hat. Frauen leisten viel mehr Pflegearbeit, sowohl für Kinder als auch für Pflegebedürftige in der Familie: 85% der Personen, die in den letzten drei Jahren an den Einrichtungen Pflegezeit nahmen, sind Frauen. Von den Müttern nehmen 60% mehr als sechs Monate Elternzeit, bei den Vätern 60% weniger als drei Monate. Die Zahlen sprechen für sich !“*

Marta Alirangues:
„Ja, diese Zahlen sind mir bekannt. Der Anteil an Frauen in der Pflegearbeit ist deutlich höher. Jetzt beginnen viele Frauen, diesen Zeitraum in ihren Lebenslauf aufzunehmen, wenn sie z.B. ein Kind erzogen haben. Unserer Aufgabe ist es auch, entsprechend positive „Role Models“ vorzuleben sowie Verständnis und Akzeptanz zu schaffen. Darüber hinaus sollten sich Männer mehr in die Pflegeaufgaben einbringen. Zum Glück ändern sich Gesellschaft und Wissenschaft in dieser Hinsicht, aber zu langsam.“

Thomas Schröder:
„Das IKZ hat als unterstützende Maßnahme den Dienstleister benefit@work an der Seite. Über Telefonberatung kann hierzu Expertise eingeholt werden. Es bietet eine gute Möglichkeit für die Beschäftigten, kostenfreie Informationen zu den Themen Pflege, Betreuung etc. einzuholen. Eine andere gute Sache ist die ***Zertifizierungen der Leibniz-Einrichtungen*** *(Grundsatz 5). Die Zertifizierung z.B. durch das Audit Berufundfamilie bietet eine gute Möglichkeit, mit unterschiedlichen Gruppen im Haus zu sprechen, den Stand zu erfassen, Probleme zu erkennen und Zielvereinbarungen zu definieren. Das IKZ durchläuft aktuell die Rezertifizierung und wir konnten anlässlich dieses Prozess viele wichtige Gespräche im Hause mit verschiedenen Bereichen führen. Bedingt durch die Covid-19 Erfahrungen haben die IT-gestützten Möglichkeiten des mobilen Arbeitens hier wesentlich an Bedeutung für die Beschäftigten gewonnen“.*

Thomas Schroeder dankt allen Kolleg*innen für die Zeit für das Interview und für die geleistete Arbeit im Bereich der Gleichstellung.

Thomas Schröder:
“Dear Heribert, thank you for this nice summary. Ms. Aliranguez will report to us in the FVB Board about her work & recommendations on a regular basis; the directors are required to support her accordingly. Well, let me move on to the next Principle 4, focussing on ***reconciling work and family life****. Women provide much more care work, both for children and for family members in need of care: 85% of persons taking care leave at institutions in the last three years are women. Among mothers, 60% take more than six months of parental leave, while among fathers, 60% take less than three months. These figures speak for themselves!”*

Marta Alirangues:
“Yes, I am aware of these figures. The proportion of women providing care is notably higher. A lot of women are now beginning to include this period in their CVs, for example, if they have raised a child. It is also our task to establish positive role models and to create understanding and acceptance. Additionally, men should become more involved in caregiving tasks. In this respect, society and science are fortunately changing, but alas too slowly.”

Thomas Schröder:
“The IKZ could win the service provider benefit@work as a supporting measure. Via telephone consulting, expertise can be obtained. It offers a good opportunity for employees to obtain free information on issues such as care, support, etc. ***Certification of Leibniz institutions*** *(Principle 5) is another good thing. The certification, e.g. by the Audit Berufundfamilie (work and family audit), offers a good opportunity to talk to different groups in the Institute, to determine the status, to identify problems and to define target agreements. At present, the IKZ is being recertified, and on this occasion, we have had many important talks with various departments in our Institute. Due to the Covid 19 experience, IT-supported mobile working options have considerably gained in importance for the employees”.*

Thomas Schroeder would like to thank all colleagues for taking the time for the interview and for the work done in the field of equality.

Das neue Foyer

Nach der Fertigstellung der Bauarbeiten in 2020 kann das Institut nun seine Gäste und Beschäftigten in einem neuen Eingangsbereich begrüßen. Das Foyer wurde komplett neu gestaltet – offen und hell und lädt nun zu einem Gedankenaustausch bei einem Kaffee oder Tee ein.

Besucher können sich über ein großes Display einen Einblick in die Forschung des Instituts verschaffen und über dessen Beitrag zu den Herausforderungen unserer modernen Gesellschaft, beispielsweise in den Bereichen saubere und effiziente Energie, Gesundheit, Kommunikation oder Mobilität. Es ermöglicht uns zudem wissenschaftliche oder Lehrvorträge abzuhalten, zum Beispiel für die zahlreichen Schülerinnen und Schüler von Berliner Schulen, die das Institut jedes Jahr besuchen. In Zukunft wird eine Ausstellung die Präsentation unserer Forschungsthemen ergänzen.

Neben einer schönen und angenehmen Atmosphäre bietet das Foyer nun auch genügend Platz für Veranstaltungen, insbesondere für das Catering. Als nächstes ist geplant, buchstäblich auch unsere Türen zu öffnen und das Foyer um eine Außenterrasse zu erweitern.

The new foyer

With the construction works finally completed in 2020, the institute can now welcome guests and employees in a new entrance area. The foyer has a completely new design – open and bright and invites to exchange ideas over a coffee or tea.

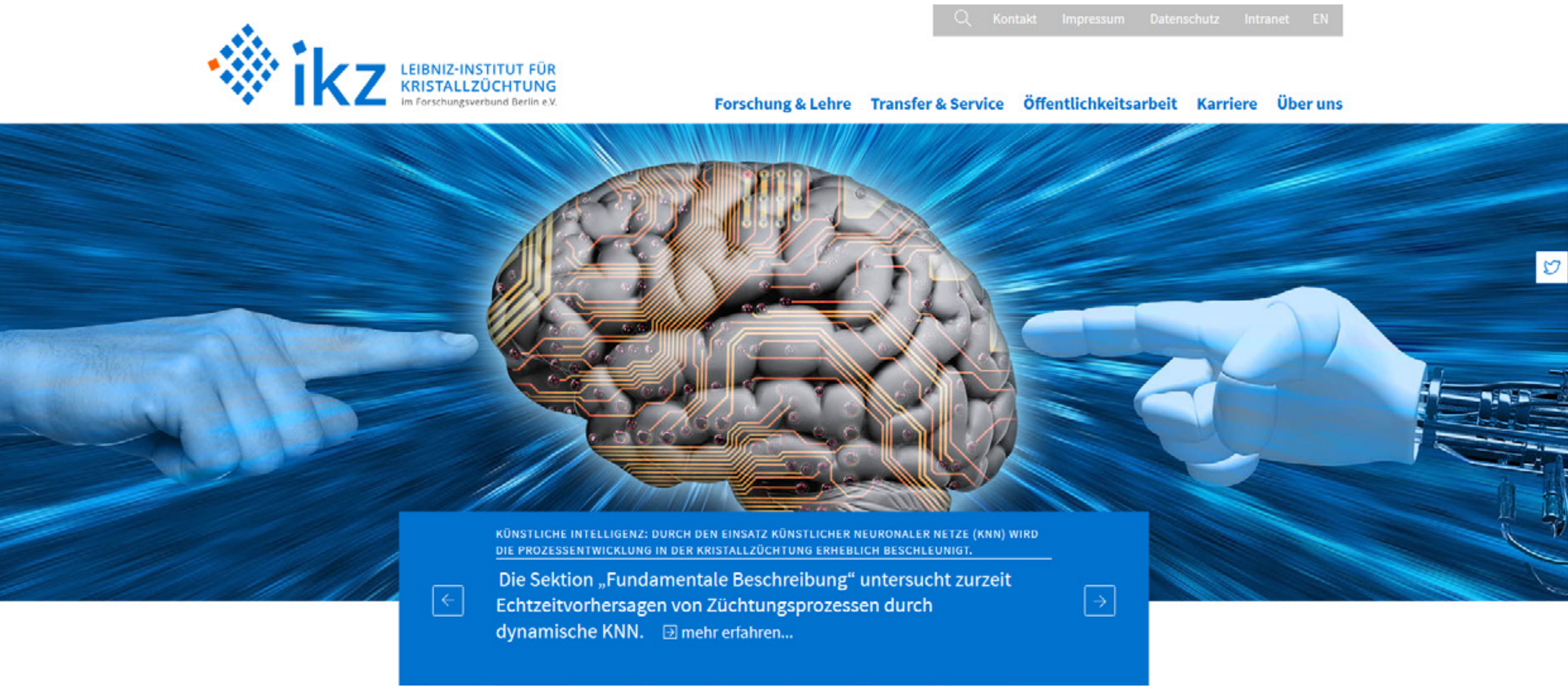
Visitors are able via a large display to get an insight into the institute’s research and its impact on challenges modern society faces today in areas like clean and efficient energy, health, communication or mobility. It also allows us to give educational presentations, for example to the numerous students from Berlin schools which are visiting the institute every year. In future, an exhibition will complement the presentation of our research topics.

In addition to a nice and pleasant atmosphere, the foyer offers now enough space for events, especially for the catering. Our next plans are literally open our doors and to expand the foyer with an outdoor terrace.

The Institute

Photo: Sebastian Rost Fotografie

Photo: Sebastian Rost Fotografie



Das IKZ präsentiert sich in neuem Online-Look

In Zusammenarbeit mit der Firma ‚Kaiserwetter‘ realisierte das IKZ 2020 eine komplette Neuaufsetzung seines Webauftritts. Der Besucher erhält direkt auf der Startseite Informationen zu aktuellen Forschungsthemen, Neuigkeiten aus den einzelnen Sektionen, Publikationen, Veranstaltungen oder Stellenangeboten des Instituts. Neben der Darstellung der IKZ Forschungsprogramme sowie dessen Forschungsstrategie finden Interessenten nun ebenso Informationen zu unseren Joint Labs & Support Labs. Zudem wird unseren Nachwuchswissenschaftlerinnen und Nachwuchswissenschaftlern nun Möglichkeit gegeben, sich nach außen zu präsentieren.

IKZ with a new online look

In collaboration with the company ‘Kaiserwetter’, a complete relaunch of the IKZ website was realized in 2020. Directly on the homepage the visitor is provided with information on current research topics, news from the individual sections, publications, events or job offers at the IKZ. In addition to the presentation of the IKZ research programs and its research strategy, now interested parties can also find information on our joint labs and support labs. The new website also offers young IKZ researchers the opportunity to present themselves to the public.

Dokumentarfilm mit IKZ Beteiligung: „Jan Czochralski – Forefather of Electronics"

Im Rahmen des Bildungsauftrages des polnischen Kulturministeriums, dem Polnischen Nationalfernsehen TVP sowie Domino Films wurde im Frühjahr 2020 unter der Leitung von Katarzyna Trzaska eine Filmproduktion zum Leben von Jan Czochralski realisiert, für die unter anderem auch Dreharbeiten am IKZ stattfanden.

Prof. Dr. Matthias Bickermann erläuterte den Fernsehzuschauern die bedeutende Rolle Czochralskis in der Geschichte der Halbleitertechnik. Jan Czochralski ist der Erfinder der bekannten „Czochralski-Methode" zur Züchtung von Einkristallen. Auch heutzutage noch werden weltweit auf diese Weise Kristalle gezüchtet, z.B. Silizium-Einkristalle für Mikroprozessoren.

Der Dokumentarfilm wurde erstmal am 3. Februar 2021 im polnischen Nationalfernsehen ausgestrahlt.

A documentary film with IKZ involvement: "Jan Czochralski – Forefather of Electronics"

In the context of the educational mission of the Polish Ministry of Culture, the Polish National Television and Domino Films, a film production about the life of Jan Czochralski was realized in spring 2020 under the direction of Katarzyna Trzaska. One of the filming locations was at the IKZ.

Prof. Dr. Matthias Bickermann gave the TV audience an insight into Czochralski's significant role in the history of semiconductor technology. Jan Czochralski invented the well-known "Czochralski method" for growing single crystals. Worldwide, crystals are still grown using this method, such as silicon single crystals for microprocessors.

The documentary was first broadcasted on Polish National Television on 3 February 2021.

Veranstaltungen
Events

12. IKZ Sommerschule: Fundamentals of Vapor-Phase Thin Film Deposition

Die Online-Variante der IKZ Sommerschule zog in diesem Jahr 45 TeilnehmerInnen aus 5 Ländern an. Für die Teilnehmenden bot die Online-Konferenz eine unkomplizierte Möglichkeit, trotz der pandemiebedingten Umstände den Sessions von Prof. Dr. Ya-Hong Xie und dem Wissensaustausch über die Dünnschichtabscheidung aus der Gasphase zu folgen.

Neben elementarer Thermodynamik und Abscheidungstechniken wurde insbesondere auf ausgewählte Themen zur Anwendung von dünnen Schichten eingegangen: Hierzu gehörten z.B. maßgeschneiderte Schichtsysteme für „Strain Engineering" in der Halbleiter-Technologien sowie Schichtanwendungen in der Mikrowellen-5G & 6G-Kommunikation.

Der studierte Physiker und promovierte Elektrotechniker Prof. Dr. Ya-Hong Xie arbeitet an der Fakultät „Materials Science and Engineering" wder University of California Los Angeles (UCLA/USA) und fokussiert seine Forschung heute vor allem im Bereich der Plasmonenresonanz sowie neuronaler Netzwerke für die Biosensorik. Dank seines vielfältigen Forschungsinteresses und umfangreichen Wissens – er war viele Jahre ein leitendes Mitglied der Bell Labs in New York – konnte er dem Auditorium eine große Bandbreite zum Stand der Forschung sowie des Anwendungsbereiches vermitteln.

12th IKZ Summer School: Fundamentals of Vapor-Phase Thin Film Deposition

This year, 45 participants from 5 countries joined the online format of the IKZ Summer School. Despite the pandemic-related circumstances, the online conference offered an uncomplicated way to follow the sessions of Prof. Dr. Ya-Hong Xie and allowed the auditorium to participate in the exchange of knowledge on vapor phase thin film deposition.

In addition to elementary thermodynamics and deposition techniques, selected topics on the application of thin films were discussed in particular: These included tailored layers for strain engineering in semiconductor technologies as well as applications of layer systems in microwave 5G & 6G communication.

Prof. Dr. Ya-Hong Xie, who studied physics and holds a doctorate in electrical engineering, works in the Department of Materials Science and Engineering at the University of California Los Angeles (UCLA / USA). Today, he focusses his research mainly in the field of plasmon resonance as well as neuronal networks for biosensor technology. Due to his diverse research interests and extensive knowledge – he was for many years a leading staff member at Bell Labs in New York-, the auditorium was given a wide range of insights on the state of the art in research & applications of this important field.

2. IKZ Winterschule: Synergy of Experimental and Numerical Studies for Crystal Growth of Bulk Semiconductors

Auch unsere IKZ Winterschule konnte im online Format einem breiten Publikum präsentiert werden. Insgesamt 54 Interessierte aus 9 Ländern folgten dem weltweit renommierten Wissenschaftler Prof. Dr. Koichi Kakimoto von der Kyushu Universität, Japan, als er über Kristallzüchtung referierte.

Die Vorträge führten die Teilnehmerinnen und Teilnehmer in allgemeine Themen ein, darunter die Anforderungen an Halbleiter aus der Geräte- und System Community oder generell Kristallzüchtungsverfahren wie CVD, PVT und andere. Insbesondere die Vertiefungen wie die 2D- und 3D-numerische Berechnung, der Stand der Technik in der Halbleitertechnologie (vor allem in Asien/ Japan und China) sowie neue Ansätze der Halbleiterzüchtung bei neuen Bauelementen führten zu spannenden Diskussionen und neuen Fragestellungen.

Koichi Kakimoto ist derzeit Professor an drei Universitäten: der Miyazaki Universität (seit 2009), der Tohoku Universität (seit 2004), und der Kyushu Universität (seit 2003). Darüber hinaus ist er Direktor des Forschungsinstituts für Angewandte Mechanik an der Kyushu Universität und Vorsitzender der IOCG (International Organization for Crystal Growth). Er ist Autor von über 350 wissenschaftlichen Publikationen.

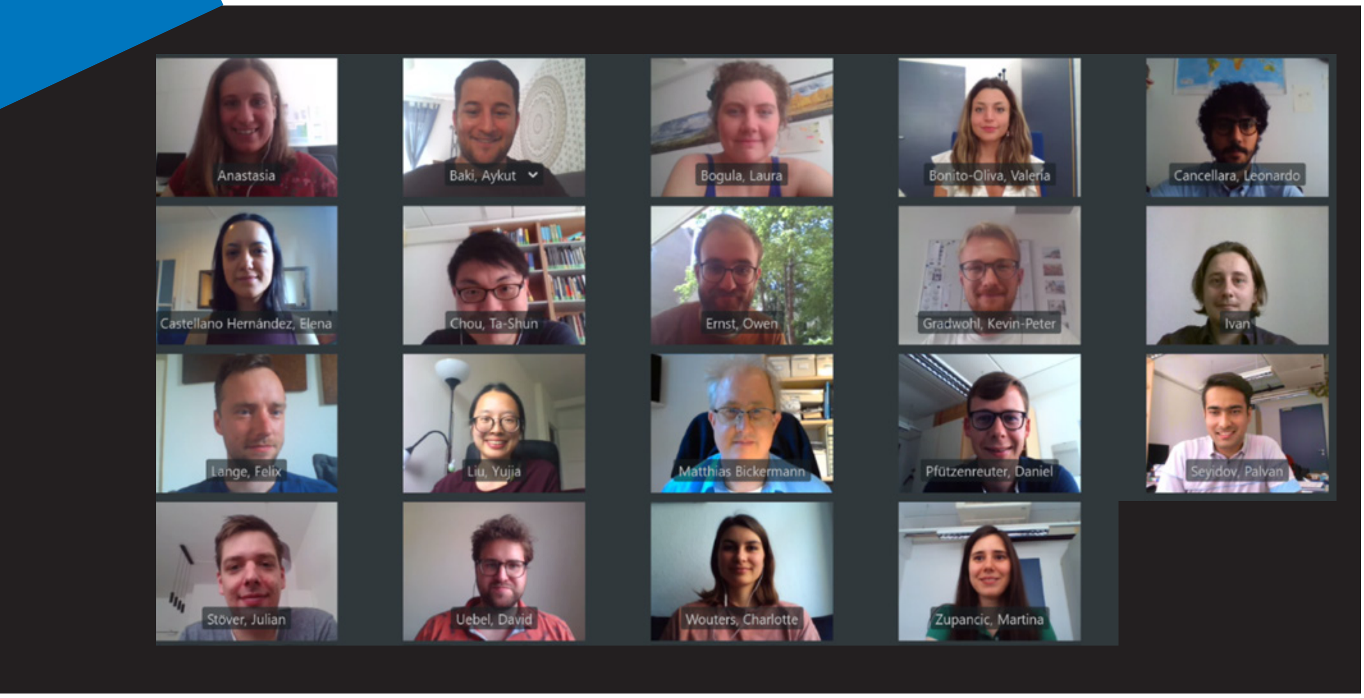
2nd IKZ Winter School: Synergy of Experimental and Numerical Studies for Crystal Growth of Bulk Semiconductors

Our IKZ Winter School could also be presented to a wide audience via online format. A total of 54 interested scientists from 9 countries were able to follow the world-renowned scientist from Kyushu University, Japan, Prof. Dr. Koichi Kakimoto, as he spoke about crystal growth.

The lecture introduced the participants to general topics such as the requirements from the device and system community on semiconductor crystals or to crystal growth processes like CVD, PVT, and others. In particular, topics such as 2D and 3D numerical calculation, the state of the art in semiconductor technology (especially in Asia/Japan and China), new approaches to semiconductor growth as well as crystal growth for new devices led to exciting discussions and scientific questions.

Koichi Kakimoto is currently professor at three universities: Miyazaki University (since 2009), Tohoku University (since 2004), and Kyushu University (since 2003). In addition, he is director of the Research Institute of Applied Mechanics at Kyushu University and Chairman of the IOCG (International Organization for Crystal Growth). He is the author of over 350 scientific papers.

Nachwuchs
Young Talents



Bericht der Promovierenden

Die Doktoranden des IKZ ließen sich auch durch die Einschränkungen durch Covid-19 Pandemie nicht beirren und nutzen die viele Zeit im Home-Office zur Optimierung ihrer schriftlichen Arbeit. Mark Edwards von der Kompetenzia International leitete ein zweitägiges Seminar mit Schwerpunkt „Completing your dissertation". Mark ist hauptberuflich Coach für führende Kräfte in Industrie und Wissenschaft und versteht es jungen Wissenschaftlern die richtigen Einblicke und Impulse zu geben, um sie auf die anstehenden Herausforderungen nach der Doktoranden-Zeit bestens vorzubereiten.

Im diesjährigen Seminar wurde besonders Augenmerk darauf gelegt die Effizienz und Struktur innerhalb der Schreibphase der Doktorarbeit zu maximieren. Wie fängt man an eine Doktorarbeit zu schreiben? Wie integriert man das Schreiben in den Arbeitsalltag? Wie behält man den roten Faden immer bei? Die Einführung in wichtige Techniken aus den Bereichen Projektmanagement und Konfliktmanagement half jedem Doktoranden dabei seinen eigenen individuellen Weg zu finden diese Fragen für sich zu beantworten.

Die Resonanz zum Workshop fiel durchgehend positiv aus und viel Erlerntes konnte von Doktoranden in der Schreibphase erfolgreich umgesetzt werden.

Report of the PhD students

The PhDs in IKZ were not disturbed by the restrictions of the Covid-19 pandemic and they efficiently used the home office to optimize their thesis writing. In last summer, Mark Edwards from Kompetenzia International gave the PhDs a two-day Seminar about "Completing your dissertation". Mark is a full-time coach for leading figures in industry and science and he knows how to give the young scientists the right insights and impulse to fully prepare themselves for the coming challenges after their PhD studies.

In the seminar, the focus was put on maximizing the efficiency and the structure within the writing phase of the PhD thesis. How to start writing a PhD thesis? How to integrate the writing into the daily working? How to keep the read thread? The guide to important techniques on the project management and conflict management helped every PhD to find his own way to answer these questions.

The response to this seminar was consistently positive and many PhDs successfully applied the techniques learned from Mark into their writing phase.

Ausgewählte Projekte
Featured Projects

Nachwuchsgruppe Multiskalen-Bildgebung mit Synchrotronstrahlung

Im April 2019 wurde die Nachwuchsforschergruppe am Leibniz-Institut für Kristallzüchtung (IKZ) im Bereich der Materialcharakterisierung mit Röntgenstrahlung etabliert. Seitdem wird sie von Dr. Carsten Richter aufgebaut und thematisch mit Leben gefüllt. Der wissenschaftliche Fokus der Gruppe liegt auf der Nutzung und Entwicklung bildgebender Röntgenverfahren im Beugungskontrast ("X-ray diffraction imaging" – XDI), wie sie vor allem an Synchrotronstrahlungsquellen verfügbar sind.

Synchrotronstrahlung ist nichts anderes als elektromagnetische Strahlung mit einem sehr breiten Spektralbereich der Röntgenstrahlung, aber auch sichtbares Licht einschließt. Die Differenzierung zwischen der für uns interessanten Röntgenstrahlung und Synchrotronstrahlung begründet sich auf den herausragenden, Laser-ähnlichen Eigenschaften der letzteren: sie ist stark gerichtet, gepulst, hochintensiv und heutzutage auch zunehmend kohärent. Synchrotronstrahlungsquellen durchliefen in den letzten Jahrzehnten eine exponentielle Steigerung bezüglich ihrer Leuchtkraft. Darüber hinaus ermöglichen neue Optiken eine Bildgebung im Nanometer-Bereich und kurze Pulse einen Einblick in Prozesse mit Pikosekunden-Dynamiken. Dadurch entstand eine Unmenge von möglichen Anwendungen in verschiedensten Bereichen. Neben lebenden Organismen, Mumien oder van Gogh-Gemälden finden sich auch Kristalle des IKZ als Proben im Synchrotron-Strahl wieder. Insbesondere mit Röntgenbeugung können atomare Struktur und Gitterdefekte im Kristall hochsensitiv untersucht werden. Der größte Nachteil der Synchrotronstrahlung ist wohl die begrenzte Verfügbarkeit: Ausschließlich an spezialisierten Teilchenbeschleunigern können nach erfolgreicher Beantragung für einige Tage Experimente durchgeführt werden. Diese laufen dann 24h am Tag und stellen immer eine besondere Herausforderung für die Nutzer-Teams dar. Besonders seit Beginn der Covid Pandemie ist die Planung und Durchführung noch komplexer, da die Versuche zum Großteil ferngesteuert vom heimischen Arbeitsplatz stattfinden.

Nach seinem Physikstudium an der TU Dresden hatte Carsten Richter an verschiedenen Synchrotronstrahlungsquellen wie dem DESY (Hamburg) und dem ESRF (Grenoble) die Gelegenheit experimentelle Methoden und Aufbauten kennenzulernen und zu entwickeln. Sein Fokus lag dabei immer auf Struktur und Symmetrie von kristallinen Materialien.

Junior Research Group "multi scale imaging using synchrotron radiation"

In April 2019, a new junior research group in the field of materials characterization using X-rays has been established at the Leibniz-Institut für Kristallzüchtung (IKZ). Since then, Dr. Carsten Richter is leading the group and develops its research topics. The scientific focus of the group lies with the use and development of X-ray diffraction imaging (XDI), a technique that is mainly available at synchrotron radiation sources.

Essentially, synchrotron radiation is nothing else than electromagnetic radiation with a very broad spectral range that includes X-rays but also visible light. The differentiation between X-rays, which are of interest to us, and synchrotron radiation is based on the latter's outstanding laser-like properties: it is highly directional and intense, pulsed, and nowadays also increasingly coherent. Synchrotron radiation sources have undergone an exponential increase in brightness over the last decades. In addition, new optics enable imaging at the nanometer scale and short pulses provide insight into processes with picosecond dynamics. This has resulted in a plethora of potential applications in a wide variety of fields. Besides living organisms, mummies or van Gogh paintings, samples in the synchrotron beam do also include crystals of the IKZ. Especially with X-ray diffraction, atomic structure and lattice defects in the crystal can be investigated in a highly sensitive way. The biggest disadvantage of synchrotron radiation is probably its limited availability: Experiments can only be carried out at specialized particle accelerators for a few days after a successful application. Then they run 24 hours a day and always present a special challenge for the user teams. Especially since the beginning of the Covid pandemic, the planning and execution is even more complex, as most of the experiments are performed remotely from the home workstation.

After his physics studies at the TU Dresden, Carsten Richter had the opportunity to get to know and to develop experimental methods and setups at different synchrotron radiation sources like DESY (Hamburg) and ESRF (Grenoble). His focus was always on structure and symmetry of crystalline materials. "The work at the IKZ now offers me the opportunity to use my knowledge in practice to illuminate current problems in materials development with synchrotron radiation," says Carsten Richter, "and to design tailored methods or experiments.

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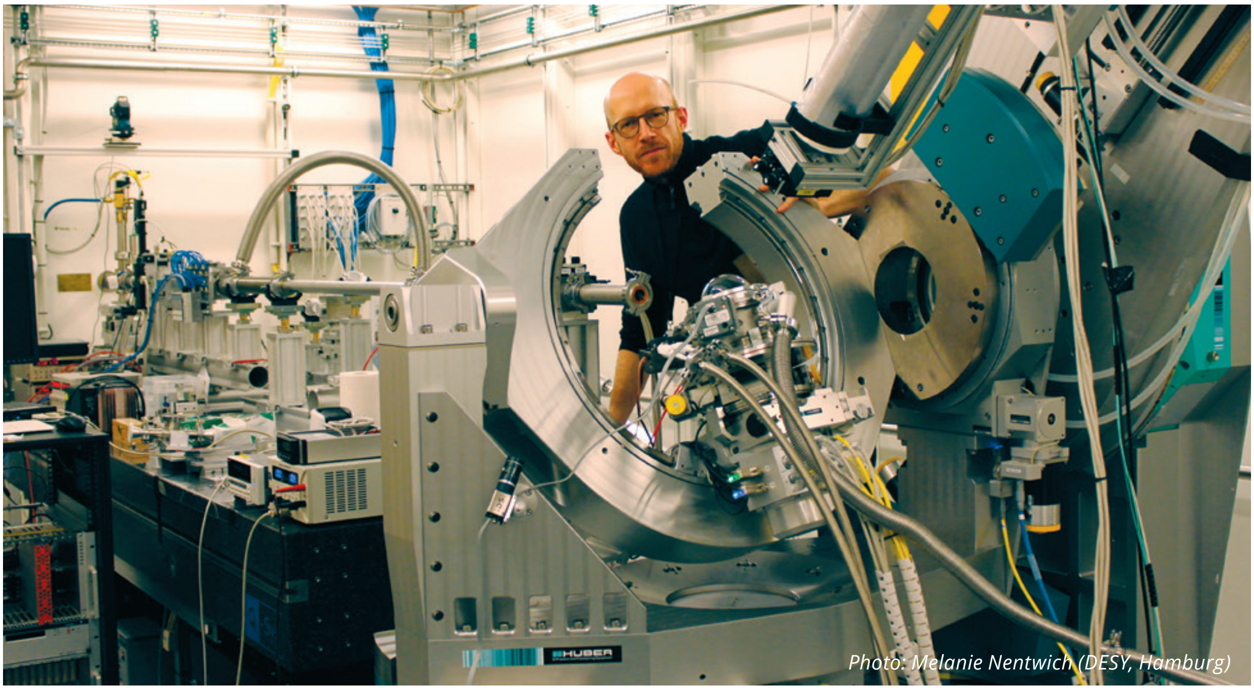

Photo: Melanie Nentwich (DESY, Hamburg)

Carsten Richter am Diffraktometer der „in-situ X-ray diffraction and imaging beamline“ P23 des DESY (Hamburg)
Carsten Richter at the diffractometer of the “in-situ X-ray diffraction and imaging beamline” P23 at DESY (Hamburg)

„Die Arbeit am IKZ bietet mir jetzt die Gelegenheit meine Kenntnisse praktisch zu nutzen um aktuelle Fragestellungen der Materialentwicklung mit Synchrotronstrahlung zu beleuchten“, sagt Carsten Richter, „und zugeschnittene Methoden oder Experimente zu konzipieren. Die vielseitigen Themen am IKZ sind reizvoll, weil ich einen tieferen Einblick in dahinterstehende Anwendungen gewinnen kann und für die verschiedenen wissenschaftlichen Probleme unterschiedlichste Messansätze in Betracht kommen. Auch der engere Kontakt zu anderen Charakterisierungsgruppen ist sehr bereichernd und weitet den Blick auf Methoden abseits der Synchrotronstrahlung“.

Eine Herausforderung in der Anfangsphase am IKZ war zunächst die Vernetzung mit anderen Forschungsgruppen und Kollegen aus unterschiedlichsten Wissenschaftsgebieten um konkrete Themen für Forschungsprojekte festzustellen. Die Züchtung von einkristallinen Materialien liegt am IKZ im Fokus von Forschung und Entwicklung. Der Anspruch der Charakterisierung ist es, unser Verständnis dieser Materialien und besonders des Zusammenhangs ihrer Eigenschaften mit Struktur und Wachstums zu verbessern, und auf diesem Wege damit verbundene wissenschaftliche Fragestellungen aufzuklären. So entstanden Aktivitäten vor allem im Bereich der Abbildung von Defekten und Verzerrung im Kristallgitter auf verschiedenen Größenordnungen und in verschiedenen Materialsystemen. Dazu zählen beispielsweise SiGe-Heterostrukturen und daraus gefertigte Quanten-Bits, Aluminiumnitrid als Substratmaterial oder III-Nitride generell als epitaktischer Film, sowie Massivkristalle und Schichten von Oxiden für elektronische Anwendungen.

The versatile topics at the IKZ are appealing because I can gain a deeper insight into underlying applications and a wide variety of measurement approaches can be considered for the various scientific problems. Also the close contact to other characterization groups is very enriching and broadens the view on methods beyond those based on synchrotron radiation".

One challenge in the initial phase at the IKZ was to network with other research groups and colleagues from a wide variety of scientific fields in order to identify concrete topics for research projects. The growth of single crystalline materials is the focus of research and development at the IKZ. The aim of characterization is to improve our understanding of these materials and especially of the correlation of their properties with structure and growth, and in this way to elucidate related scientific issues. Thus, activities have emerged mainly in the area of imaging defects and strain in the crystal lattice at different scales and in different material systems. These include, for example, SiGe heterostructures and quantum bits fabricated from them, aluminum nitride as a substrate material or III-nitrides in general as an epitaxial film, as well as bulk crystals and layers of oxides for electronic applications.

Neutrinos und Gravitationswellen – unser Beitrag zur Erforschung des Kosmos

Das Verständnis der Entstehung des Universums beginnt mit der Erforschung seiner Grundbausteine (und damit auch der unserer Existenz) und ihrem Verhalten unter extremen physikalischen Bedingungen. Verschiedene experimentelle Ansätze versuchen die Dynamik von Galaxien und die Bausteine des Universums als Ganzes zu untersuchen. Sie berühren dabei viele Fachgebiete der Physik wie die Kosmologie oder die Hochenergie-Astroteilchenphysik mit dem Ziel die Fragen nach der Natur der komplexen astrophysikalischen Phänomene wie die Entstehung von Schwarzen Löchern, Neutronensternen, Dunkler Materie, Gravitationswellen oder der Materie-Antimaterie aufzuklären. Kristalline Materialien können eine fundamentale Rolle in diesen Untersuchungen spielen, entsprechend ist das IKZ an Kosmologie Forschungsprojekten beteiligt, in Kooperationen mit nationalen und internationalen Partnern. Aktuell wird diese interessante Grundlagenforschung durch zwei Projekte (LEGEND und 3G-GWD-ET) unterstützt, die vom BMBF im Rahmen der Förderlinie „Erforschung von Universum und der Materie“ gefördert werden.

2015 gelang erstmalig die Beobachtung von Gravitationswellen am Laser-Interferometer Gravitationswellen-Observatorium LIGO, eine Entdeckung, die in 2017 mit dem Nobelpreis gewürdigt wurde. Das Einstein-Teleskop (ET) ist ein europäisches Gravitationswellen-Observatorium der 3. Generation, das über eine noch höhere Sensitivität verfügen wird. Mit seiner Hilfe wird es möglich sein, Präzisionsstudien der Struktur von Neutronensternen durchzuführen, von der Geburt Schwarzer Löcher oder dem Zustand des Universums unmittelbar nach dem Urknall. Ein hohes Signal-to-Noise-Verhältnis erlaubt sowohl Untersuchungen von erweiterten Gravitationstheorien und Extradimensionen, als auch von Dunkler Materie und Dichteparametern Dunkler Energie. Konzipiert als unterirdische Anlage mit mehreren Interferometern bei kryogenen Temperaturen wird das ET Gravitationswellen mit Frequenzen herunter bis zu ~ 2 Hz detektieren können. Ein entscheidender Aspekt der Konstruktion des ET ist das Aufhängungssystem für die großen Interferometer-Spiegel. Jeder dieser ca. 200 kg schweren Spiegel wird von Fasern von 1–1,5 m Länge und nur wenigen Millimetern im Durchmesser gehalten. Kristallines Silizium ist mit seinen für diesen Zweck fast perfekten mechanischen und thermischen Eigenschaften das Material der Wahl für diese Fasern.

Neutrinos and gravitational waves – our contribution to cosmic exploration

The quest for understanding the origin of the universe starts with studying the basic building blocks of the universe (and also of our existence) and their behaviours under extreme physical conditions. There are different experimental approaches to study the dynamics of galaxies and the constituents of the universe as a whole. It touches many physics subject areas like cosmology or high-energy astro-particle physics to address directly the questions about the nature of complex astrophysical phenomena such as formation of black holes, neutron stars, dark matter, gravitational waves or matter-antimatter existence. Since crystalline materials can play a fundamental role in these investigations, IKZ is also involved in cosmology-related research in co-operation with national and international partners. Two projects (LEGEND and 3G-GWD-ET) funded by BMBF in 2020 within the framework of the funding program “Exploration of the universe and matter“, support this interesting fundamental research.

The observation of gravitational waves was first accomplished in 2015 at the Laser Interferometer Gravitational-Wave *Observatory Advanced LIGO*, a discovery awarded with the Nobel Prize in 2017. The Einstein Telescope (ET) is a future 3rd generation gravitational wave observatory in Europe and will be designed with even higher sensitivity. It will allow precision studies of the structure of neutron stars, the birth of black holes or the state of the universe immediately after the Big Bang. High signal-to-noise observations will allow the examination of extended gravity theories and extra dimensions, as well as the measurement of dark matter and dark energy density parameters. Designed as a new underground facility with several interferometers operating at cryogenic temperatures, the ET will be sensitive to gravitational wave frequencies down to ~ 2 Hz. A crucial aspect in the design of the ET is the suspension system for the large interferometer mirrors. Each mirror of about 200 kg weight will be held by four fibers of 1 – 1.5 m length and only a few mm in diameter. Crystalline silicon has almost perfect mechanical and thermal properties and would be an ideal material for such fibers. Especially the isotope ^{28}Si is of interest here, due to its extremely high thermal conductivity in the interferometer working temperature of T = 24.1 K. This would allow to dissipate the heat from the mirrors efficiently, which will reduce thermal noise and allow for higher laser power and sensitivity for gravitational waves.

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Insbesondere das Isotop ^{28}Si ist hier von Interesse, da es über eine extrem hohe thermische Leitfähigkeit bei der Betriebstemperatur des Interferometers bei T=24,1 K verfügt. Dies würde eine effiziente Wärmeableitung von den Spiegeln ermöglichen, d.h. eine Reduzierung des thermischen Rauschens und bedeutet damit eine höhere Laserleistung und Sensitivität für Gravitationswellen. Im Rahmen der ET-Pathfinder Kooperation befasst sich das IKZ mit der Entwicklung einer Herstellungsmethode für diese kristallinen Siliziumfasern. Für die Züchtung der versetzungsfreien Fasern mit der benötigten Reinheit kommen dabei insbesondere tiegelfreie Methoden wie Float Zone oder Pedestal in Betracht. Abb. 1 zeigt den Aufbau für die Pedestal-Züchtung, eine Silizium-Faser mit 3 mm Durchmesser während der Züchtung und das Faseraufhängungssystem im Einstein-Teleskop. Mehr über das Einstein-Teleskop findet sich unter
https://www.einsteintelescope.nl/en/.

Eine weitere große internationale Zusammenarbeit mit Beteiligung von mehr als 50 Ländern ist das Projekt LEGEND (Large Enriched Germanium Experiment for Neutrinoless Double beta decay). Diese Kooperation befasst sich mit der Entwicklung eines Experiments für die Detektion des neutrinolosen Doppelbetazerfalls (0nßß) von Germanium-76 mithilfe von Detektorenarrays aus ultra-reinen, isotopenangereicherten ^{76}Ge Einkristallen. In diesen Arrays dient das Germanium sowohl als Detektormaterial als auch als Quelle für die Zerfallsreaktionen.

In the frame of the ET-Pathfinder collaboration, IKZ aims to develop a production method for such crystalline silicon fibers. Especially crucible-free methods, such as float zone and pedestal, are suitable to grow fibers with the required high purity and free from dislocations. Fig. 1 shows the pedestal growth setup, Si fiber of 3 mm diameter during growth, and a fiber suspension system in the ET. More information on the Einstein Telescope project can be found at
https://www.einsteintelescope.nl/en/.

The Large Enriched Germanium Experiment for Neutrinoless Double beta decay (LEGEND) is another grand international collaboration with participation of more than 50 countries. This collaboration develops an experimental program to search for the neutrinoless double-beta-decay (0nßß) of ^{76}Ge, using arrays of detectors made of ultra-pure ^{76}Ge isotopic single crystals. In this setup, germanium will serve as detector material as well as source for the decay. The decay itself is extremely rare, with a half-life period $T_{1/2}$ of more than 10^{26} years, that is a billion million times the age of the universe. Evidence of such decay would not only prove that neutrinos and anti-neutrinos are identical particles, but it would also explain the lightness of neutrinos and would provide hints to why matter is so much more abundant than anti-matter in today's universe.

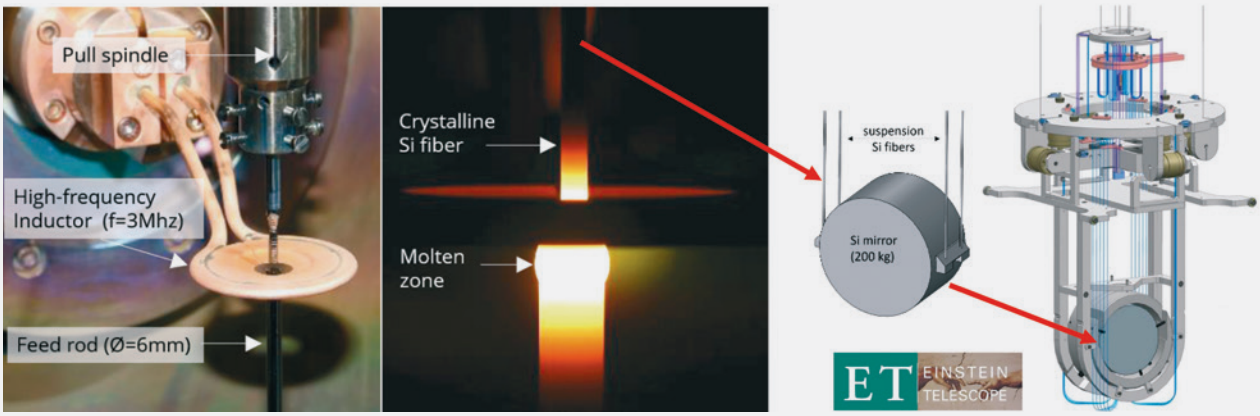

Abb. 1
Aufbau der Pedestalzüchtung für die Herstellung von Si Fasern für die Spiegelaufhängung im Einstein-Teleskop.
Links: Züchtungsaufbau,
Mitte: Züchtung einer kristallinen Si-Faser mit einem Durchmesser von 3 mm,
Rechts: Skizze der Spiegelaufhängung
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Fig. 1
Pedestal growth method for production of Si fibers for use as mirror suspensions in ET
Left: Growth setup,
Middle: Si crystalline fiber with diameter of 3 mm during growth,
Right: Mirror-suspension sketch (mirror-suspension figure is reprinted with the permission from ET Pathfinder Collaboration,
https://apps.et-gw.eu/tds/?content=3&r=17177,
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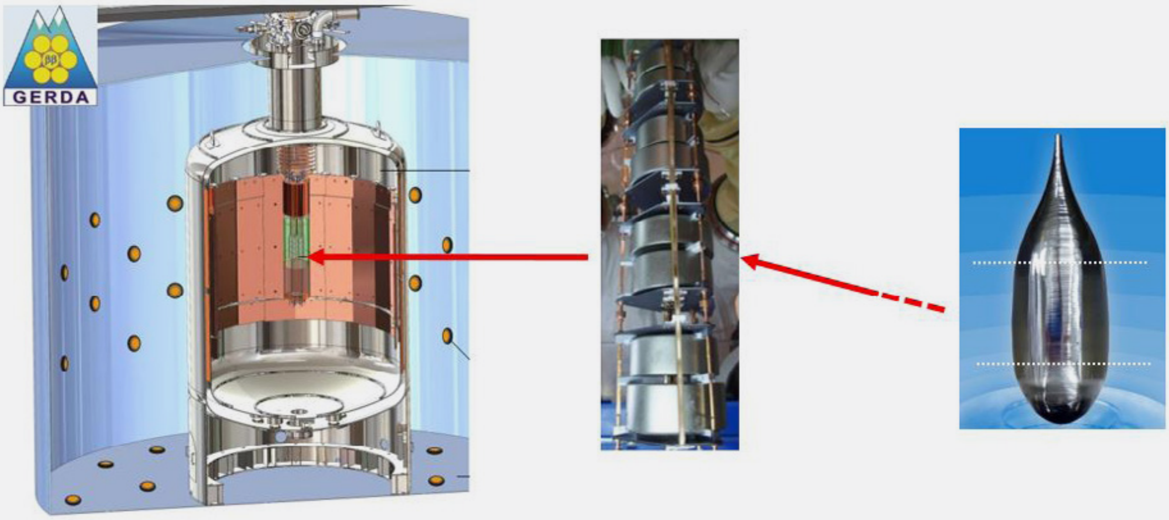

Abb. 2
Links: Skizze des experimentellen GERDA-Aufbaus (später modifiziert für LEGEND-200); Mitte: HPGE Detektor-Array (beide Abbildungen verwendet mit freundlicher Genehmigung durch die GERDA/LEGEND Kollaboration, https://legend-exp.org/science/neutrinoless-bb-decay/legend-detectors, © GERDA/LEGEND Collaboration); rechts: HPGe Kristall gezüchtet nach der Czochralski-Methode, Durchmesser ~76 mm.

Fig. 2
Left: Sketch of the GERDA experimental set-up (later modified for LEGEND-200); middle: HPGe detector arrays, Right: 76 mm diameter Czochralski-grown HPGe crystal at IKZ (Figures in the left and middle are reprinted with the permission from GERDA/LEGEND collaboration, https://legend-exp.org/science/neutrinoless-bb-decay/legend-detectors, copyright @GERDA/LEGEND Collaboration)

Der Zerfall an sich ist ein extrem seltenes Ereignis mit einer Halbwertszeit $T_{1/2}$ von mehr als 10^{26} Jahren, was mehr als eine Milliarde Millionen Mal dem Alter des Universums entspricht. Der Nachweis eines solchen Zerfalls würde nicht nur belegen, dass Neutrinos ihre eigenen Antiteilchen sind, sondern würde zudem ihr geringes Gewicht erklären und Aufschlüsse geben zu der Frage, warum es im heutigen Universum weitaus mehr Materie als Antimaterie gibt. Die ^{76}Ge Experimente der heutigen Generation (LEGEND-200) im Gran Sasso Untergrundlabor sehen den Einsatz von mehreren ^{76}Ge Detektorkristalle mit einem Durchmesser von 80 mm vor mit einer Gesamtmasse von 200 kg, die sowohl einen extrem niedrigen Hintergrund als auch eine sehr hohe Energieauflösung bieten. Auf diese Weise ist es möglich, die Sensitivität des Experiments soweit zu erhöhen, dass auch Zerfälle mit einer Halbwertszeit größer als 10^{28} Jahren detektiert werden könnten. Als Mitglied der LEGEND Kollaboration (**http://legend-exp.org**) entwickelt das IKZ die Technologien für die Züchtung von ultrareinen Germanium (HPGe) Einkristallen in „Detektorqualität", sowie für die effiziente Bearbeitung des isotopenreinen Germaniums. Abb. 2 zeigt einen unserer Kristalle, gezüchtet unter H_2-Atmosphäre mit der Czochralski Methode. Die Kristalle sollen einen Reinheitsgrad erreichen mit einer Nettoladungsträgerkonzentration von $n < 10^{10}$ cm^{-3} und einer kontrollierten Versetzungsdichte zwischen 10^2 und 10^4 cm^{-2}.

Current generation ^{76}Ge experiments (LEGEND-200) at the Gran Sasso underground laboratory plan to employ several 80 mm diameter ^{76}Ge crystalline detectors with a total mass of 200 kg, providing both ultra-low background and very high energy resolution. In this way, the sensitivity of the experiment will be enhanced to a discovery potential for a half-life period beyond 10^{28} years. As a member of the LEGEND collaboration (**http://legend-exp.org**), IKZ is developing a technology for growing "detector grade" ultra-high purity Ge (HPGe) single crystals and also for effective processing of the isotopically enriched Ge material. These crystals (shown in Fig.2 right) grown by Czochralski method under H_2 gas environment, are targeted to reach a purity level of a net carrier concentration $n < 10^{10}$ cm^{-3} with controlled dislocation density in the range of 10^2 – 10^4 cm^{-2}.

Neue Float-Zone Züchtungs-anlage für Siliziumkristalle bis zu 8 Zoll

Das Float-Zone (FZ) Verfahren eignet sich ausgezeichnet für die Herstellung von Volumenkristallen von ultrahoher Reinheit und Perfektion. Dem IKZ in Berlin steht seit 2020 eine neue FZ Anlage für die Züchtung von großen Silizium-Kristallen mit einem Durchmesser von bis zu 8 Zoll (200 mm) zur Verfügung. Das ist der bisher größte mit der FZ Methode erreichbare Durchmesser. Das IKZ kann damit seine führende Rolle im Hinblick auf die akademische und industrielle FZ Züchtung weiter ausbauen.

Größe macht den Unterschied – Wafer mit größerem Durchmesser ermöglichen Durchsatzsteigerungen bei der Herstellung elektronischer Bauelemente. Bei der Produktion von Hochleistungs-Halbleitern mit besonders niedrigem Gehalt an Fremdstoffen wie Sauerstoff und Kohlenstoff und mit sehr hohem elektrischem Widerstand ist der Wafer-Durchmesser durch das FZ Verfahren limitiert. Leistungshalbleiter finden in der gesamten Energiewertschöpfungskette Verwendung, von der Stromerzeugung, dessen Übertragung bis zur Nutzung, z.B. im Bereich Elektromobilität. In Anbetracht des Klimawandels gewinnen Leistungshalbleiter an Bedeutung, da sie nachhaltige Lösungen durch intelligentes Energiemanagement ermöglichen.

New float-Zone furnace for silicon crystals up to 8 inches

The Float-Zone (FZ) process stands out for its ability to produce volume crystals with ultra-high purity and perfection. The IKZ has acquired a new FZ furnace for the growth of large silicon crystals with a diameter of up to 8 inches (200 mm). This is so far the largest diameter that can be achieved using the FZ method. With this step the IKZ is able to strengthen its leading role in FZ academic and industrial research.

Size matters – larger diameter wafers allow for more die per wafer. In the production of high-power semiconductors with very low content of impurities like oxygen or carbon and with high electrical resistance, the wafer diameter is limited by the FZ process. Power semiconductors (IGBT, MOSFET) are used throughout the entire energy value chain, from electricity generation, its transmission to its use, e.g. in e-mobility. In consideration of climate change, power semiconductors are gaining in importance as they enable sustainable solutions using intelligent energy management.

The modern crystal growth furnace FZ-30 was funded in frame of a so called item of extraordinary expenditure ("Sondertatbestand"), and built by the company PVA TePla in Jena, Germany. The technological demands for the furnace with a height of 12 m and a total weight of 20 t are challenging. For example, during growth the silicon rods with a weight of more than 100 kg must be moved absolutely vibration-free with millimeter accuracy. In comparison to the three existing FZ furnaces at IKZ, the advanced mechanics of the FZ-30 not only allow the growth of crystals with larger diameter but also at higher process stability and with increased dopant homogeneity in the crystal. The growth chamber withstands an overpressure of the inert gas atmosphere of 3 bar. This reduces the risk of arcing at high heating power of the induction generator with a maximum capacity of 120 KW. With the help of IKZ know-how, the machine type actually designed for industrial production has been extensively modified for research operation, thus extending the available free parameter space for new FZ process development. Additional feedthroughs and process equipment as infrared heaters were added to the growth chamber. The FZ process can be operated via the completely new designed user interface or via the semi-automatic control developed at IKZ.

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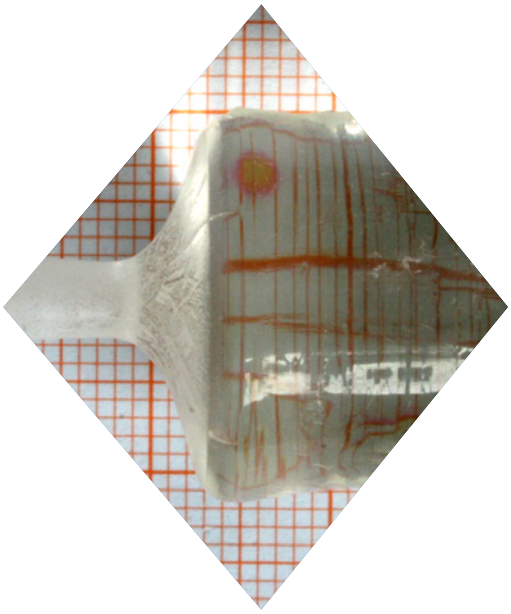
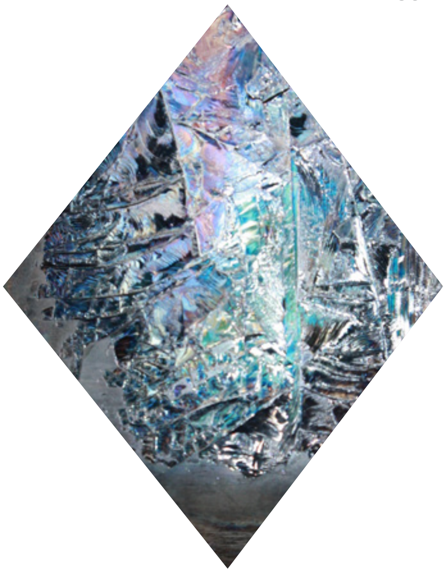
Die moderne Züchtungsanlage FZ-30 wurde im Rahmen eines Sondertatbestands finanziert und von der Firma PVA TePla AG in Jena gebaut. Die technologischen Anforderungen an die Anlage mit einer Höhe von 12m und einem Gesamtgewicht von 20t sind auch deshalb enorm, weil die Siliziumstäbe mit einem Gewicht von über 100 kg bei der Züchtung absolut schwingungsfrei und millimetergenau bewegt werden müssen. Im Vergleich zu den drei am IKZ bestehenden FZ-Anlagen erlaubt die bessere Mechanik der FZ-30 nicht nur das Ziehen größerer Kristalle, sondern auch die Züchtung mit höherer Prozessstabilität und Dotierstoffhomogenität im Kristall. In der FZ-30 kann eine Inertgas-Atmosphäre mit bis zu 3 bar Überdruck erzeugt werden. Das mindert das Risiko des elektrischen Durchschlags bei hoher Heizleistung des Induktionsgenerators bis 120 kW. Der eigentlich für die industrielle Produktion konzipierte Anlagentyp wurde mit IKZ-Knowhow für den Forschungsbetrieb umfangreich modifiziert und so der freie Parameterraum für den Prozess erweitert. Der Rezipient wurde um zusätzliche Durchführungen und Versuchseinbauten wie Infrarotheizer ergänzt. Der FZ Prozess kann über die vollständig neu entworfene Benutzerschnittstelle gesteuert oder teilweise automatisch mit der am IKZ entwickelten Regelung gefahren werden.

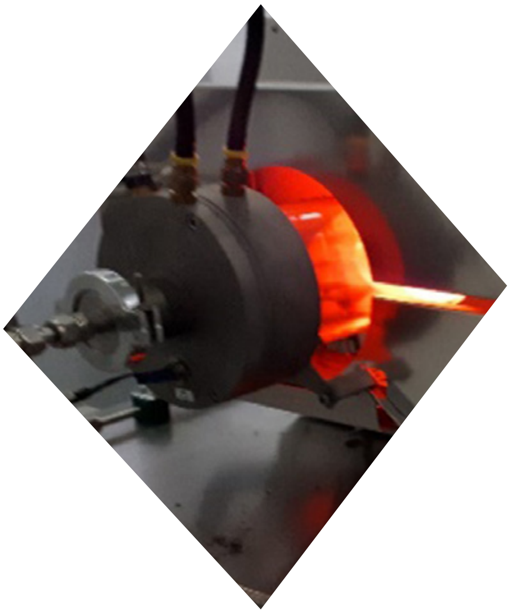
Derzeit ist das IKZ auf dem Weg, das 8-Zoll-FZ-Verfahren in Zusammenarbeit mit der Firma PVA Tepla AG zu entwickeln. Auch die Forschung zur Erreichung einiger wichtiger Kristalleigenschaften steht in enger Zusammenarbeit mit der Siltronic AG im Fokus. Zukünftig sollen mit dieser neuen Anlage FZ-30 die Prozesse für Kristalle mit sehr hoher Reinheit und Dotierstoffhomogenität für die nächste Generation der Silizium-Leistungselektronik entwickelt werden.

Für eine bessere Beherrschbarkeit des insbesondere bei großen Durchmessern komplexen FZ Prozesses sollen neue Regelungskonzepte erforscht werden.

The IKZ will now start to develop the 8-inch FZ process in close cooperation with the PVA Tepla AG. In another cooperation with the company Siltronic AG research focusses on improving some important crystal properties. For a better controllability of the FZ process especially at large crystal diameter, new automatization concepts will be investigated. In future, this new FZ-system will allow us to develop growth processes for crystals with very high purity and dopant homogeneity for the next generation of silicon based power electronics.







Volume Crystals

Volume Crystals

Requirements, growth and evaluation of GaAs cryogenic scintillator crystals

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Despite overwhelming evidence that large amounts of cold dark matter (DM) are gravitationally associated with galaxies and galactic clusters, recent large-scale experiments designed to detect nuclear recoils from DM particles with masses above 1GeV/c^2 have not yet seen a definitive signal. This has motivated designs for experiments that search for DM particles in the MeV/c^2 range, using both electron and nuclear recoils. Scintillators are promising targets for detecting DM particles due to scattering of electrons [1]. A recent evaluation of prospective cryogenic scintillation radiation detector materials revealed n-type GaAs as promising material. Since the scintillation luminosity strongly depends on the content of boron and silicon in the crystals [3], the main challenge is the growth of specifically doped GaAs single crystals.

Scintillating GaAs is an excellent target for the detection of rare, low-energy electronic excitations from interacting DM particles for various reasons, especially because the cryogenic bandgap is 1.52 eV, allowing the detection of electronic excitations from interacting DM particles as light photons of a few MeV/c^2 for electron elastic scattering [2] and a few eV/c^2 for inelastic processes [3]. Furthermore, there are no naturally occurring radio–active isotopes of Ga or As and the donor electrons do not freeze out above a free-carrier concentration of 8 x 10^{15}/cm^3. Metastable radiative states that could cause afterglow are annihilated by delocalized donor electrons, as evidenced by the lack of thermally stimulated luminescence [4]. Of great significance is also, that n-type GaAs can be grown in the form of bulk crystals.

N-type GaAs has a Fermi level close to the conduction band minimum and all electron traps are filled. It produces scintillation photons by the following steps: (1) an electronic excitation event leaves one or more holes in the valence band, (2) the valence band holes are trapped by acceptors and (3) the acceptor holes recombine radiatively with delocalized donor band electrons.

Figure 1 shows the GaAs:(Si,B) acceptor levels and emission energies identified in previous works. Four radiative acceptors associated with luminescence have been identified:
i) shallow defects, ii) boron on an arsenic site B_{As}, iii) silicon complex $Si_{Ga}V_{Ga}$, iv) the silicon complex $Si_{Ga}V_{Ga}Si_{Ga}$.
In addition, a variety of deeper acceptors (X) have been distinguished [5] that can trap valence band holes and reduce the luminosity below the theoretical limit of 220 photons/keV.

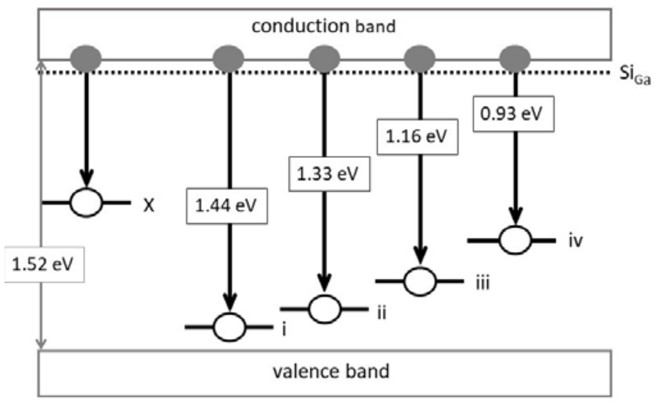

Fig. 1
The GaAs energy gap and transition energies for silicon donor electrons (Si_{Ga}) recombining with radiative acceptors i, ii, iii, iv and with non-radiative acceptors X.

In common semiconductors the n-type free carrier concentration is simply the excess of the donor concentration over the acceptor concentration. In the case of GaAs:(Si,B) the situation is more complicated. Provided that most of the boron dopants reside on isoelectronic gallium sites and that the boron acceptor emission arises from a smaller fraction of boron on an arsenic acceptor site [6], the fraction of B_{As} depends i.a. on the stoichiometric deviation of the GaAs melt and is increased in Ga-rich crystals respectively.

Volume Crystals

In order to achieve an n-type GaAs with a free carrier concentration in the range of 10^{17} cm^{-3}, a Si concentration in the order of 1-5 x 10^{17} cm^{-3} is required, as well as a significantly higher boron content (10^{18} cm^{-3} - 10^{19} cm^{-3}) to achieve B_{As} above 10^{16} cm^{-3}.

In order to optimize the complex dopant household 4 inch GaAs crystals were grown by the vertical gradient freeze (VGF) technique; Figure 2 shows a sketch of the VGF container. Under standard crystal growth conditions of VGF-GaAs, even when using B_2O_3, it is not possible to obtain the aforementioned necessary B-Si ratios in a crystal. When B_2O_3 is used as encapsulant, boron is incorporated into GaAs by an exchange reaction in the same order of magnitude as Si, but the Si content would be too high to obtain the required B content. Therefore, it is crucial to adjust the growth conditions in order to obtain GaAs crystals with point defect sites in the necessary ratios.

After optimization of the process parameters, we were able to grow GaAs with the following properties: Si doping in a range of 2-8 x 10^{17} cm^{-3} and additionally compensated by C_{As}, which is the most important acceptor in GaAs. The B concentration varies from 2 x 10^{18} to 10^{19} cm^{-3}. In this context, the influence of the water content of the used B_2O_3 on the variation of the B concentration was also investigated. Furthermore, experiments with an additional carbon source in the growth container were carried out to increase the acceptor concentration (see Fig. 2).

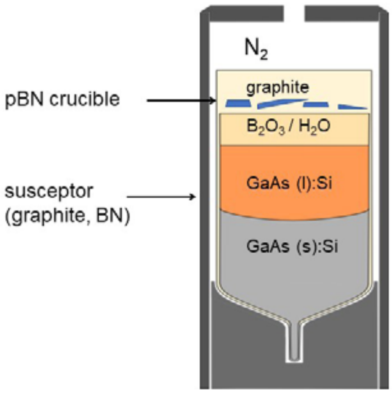

Fig. 2
Sketch of the VGF system with B2O3 encapsulation.

The total luminosities were measured as described in [3]. The most luminous VGF-GaAs sample studied has an observed scintillation luminosity of 96.2 photons/keV. The crystal from which the sample at the beginning of the cylinder was prepared is shown in Figure 3, including the measured doping concentrations, measured by SIMS.

$n \sim 4\cdot10^{17}$ cm^{-3}
$c_{Si} \sim 3\cdot10^{17}$ cm^{-3}
$c_B \sim 1\cdot10^{19}$ cm^{-3}
$c_C \sim 2\cdot10^{16}$ cm^{-3}
Grown from slightly Ga-rich melt

Fig 3
VGF-GaAs crystal with currently the highest total luminosity of 96.2 photons/keV.

These measurements show that n-type GaAs is a promising cryogenic scintillator for DM particle detection in the MeV/c^2 mass range since it can be grown as high-quality crystals and has good scintillation luminosity. However, more work is needed to optimize the delicate balance between the concentrations of different dopants, and to develop suitable cryogenic photodetectors.

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Cubic $Li_7La_3Zr_2O_{12}$: Fast Li ion conductor for next generation solid electrolytes

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A serious drawback of most renewable energy sources is limited operating lifetime and lack of reliability. A major challenge for the efficient use of renewable energy is the development of suitable electrical energy storage devices that combine high energy density with durability and safety. With the rapid increase of overall market share of fully electric zero emission vehicles and hybrid or plug-in electric vehicles, the global demand for compact mobile storage devices is expected to increase vastly. The most convenient form of electrical energy storage is electrochemical storage such as batteries and supercapacitors. Among those, rechargeable lithium ion batteries are attaining significant attention because of their high energy density compared to other battery systems.

The most promising ceramic electrolyte is garnet-type cubic $Li_7La_3Zr_2O_{12}$ (LLZO). In particular, its stability against Li-metal as well as its thermal and mechanical robustness makes LLZO garnet exceptionally well-suited to be used as a protecting layer for Li-metal-based batteries. Pure LLZO occurs in two structural polymorphs. The low-temperature tetragonal modification is characterized by a completely ordered distribution of Li ions, whereas the cubic high-temperature modification exhibits a disorder in the Li^+ distribution. The two orders of magnitude higher Li ion conductivity makes the cubic modification attractive for battery application. Stabilization of the cubic modification can be achieved by incorporating supervalent ions, e.g. Al^{3+} or Ga^{3+}, onto Li^+-sites accompanied by the creation of two vacancies in the Li-sublattice. Notably, this substitution further increases ionic conductivity: Ga-stabilized LLZO has a room temperature Li^+ conductivity of more than 1 mS/cm.

Many relevant properties of solid electrolytes are critically affected by the ‚shape' of the individual sample, e.g. grain boundaries, distribution of grain sizes, porosity etc. which may differ significantly from sample to sample. Single crystals instead provide the opportunity to investigate the intrinsic material's behaviour since they are practically free of grain boundaries, 100% dense and can be prepared with an exceptional chemical homogeneity largely excluding sample-to-sample variations. Using single crystalline specimens it becomes possible to study e.g. the influence of dopants in much greater detail or to clearly distinguish between intragrain and grain boundary effects.

We have grown LLZO single crystals with the cubic phase stabilized by Ga^{3+} or Al^{3+} doping using the Czochralski technique. Stoichiometric mixtures of the previously dried starting materials with an additional excess of 10% Li_2O were pressed and sintered at 850°C, ground, pressed, and sintered again at 1230°C. This is the standard procedure used in preparation of ceramic samples and believed to yield single phase LLZO polycrystalline solids – perfect compacted starting material for the growth. This material was melted in a 40 ml sized, inductively heated iridium crucible placed in a thermal cavity made of alumina insulation. To protect the iridium crucible from oxidation, the entire thermal cycle was carried out in inert atmosphere. Growth was accomplished using the automatic diameter control facility based on crucible weight change. A great challenge is connected with the volatility of Li_2O at working temperature and etching of the growing crystal in a Li_2O-rich ambient. On the one hand, Li loss of the melt must be compensated by an appropriate excess in the starting composition. On the other hand, the thermal profile in the setup must be designed to minimize evaporation and recondensation of Li_2O on the growing crystal.

Volume Crystals

The grown LLZO crystals were around 15 mm in diameter and up to 40 mm long. Typically, the crystals showed a degraded surface in their upper, first grown part and a smooth and shiny surface in the bottom part (Fig. 1) with the interior mainly free of coarse defects. From theses crystal appropriate samples could be prepared for investigations.
In the reporting period, two studies were published in cooperation with our partners at the Graz University of Technology (now at NTNU Trondheim). The first focusses on self-discharge and internal short circuits in batteries evoked by Li dendrites. It had been suggested that even a very low electronic conductivity can animate the formation of Li dendrites in LLZO-type garnets. The values of the electronic conductivity published by different groups working with ceramic samples differ by some orders of magnitude. We probed the electronic and ionic conductivity of single crystalline $Li_{6.4}Ga_{0.2}La_3Zr_2O_{12}$ by means of broadband impedance spectroscopy and potentiostatic polarization and estimated an upper limit for the electronic conductivity at room temperature of the order of 5×10^{-10} S/cm. This is at least six orders of magnitude lower than the Li-ion conductivity.

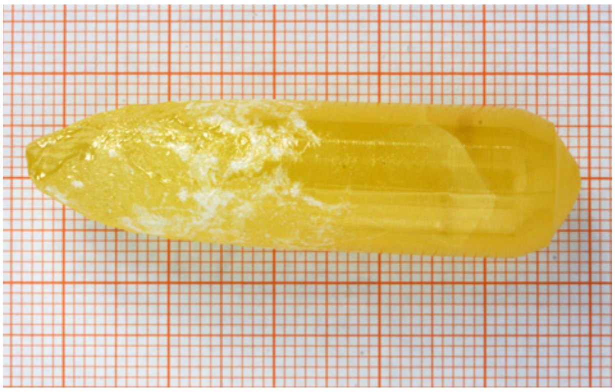

Fig. 1
LLZO ($Li_{6}.4Ga_{0}.{}_{2}La_3Zr_2O_{12}$)
single crystal grown by the Czochralski technique.

The second paper studies the critical current density in symmetrical Li-metal cells (see Fig. 2). Based on galvanostatic cycling experiments and impedance spectroscopy, an exponential dependence of the critical current density on the area specific resistance was observed in single crystalline $Li_{6.4}Ga_{0.2}La_3Zr_2O_{12}$. Since single crystals have less defects as compared to polycrystalline material, the critical current density value of approximately 300 μA/cm^2 obtained represent the upper limit for $Li_7La_3Zr_2O_{12}$ at room temperature without applying external forces. This result suggests that either pressure or a significant increase in the interfacial area is needed to reach current densities larger than 3 mA/cm^2, which are necessary to realize high power all-solid-state batteries for next generation electric cars.

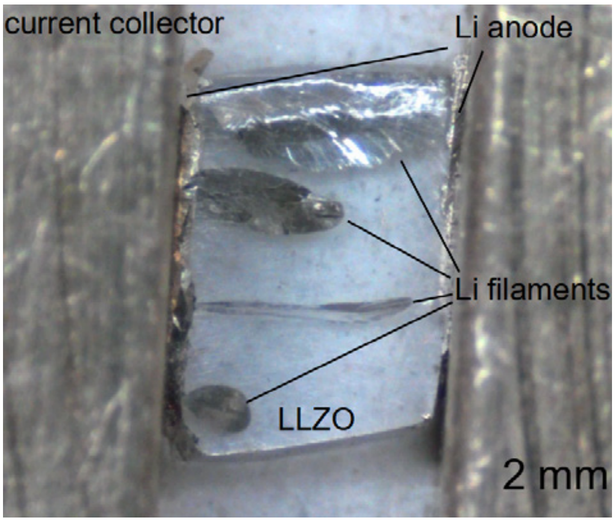

Fig. 2
Li metal penetration through a LLZO ($Li_{6.4}Ga_{0.2}La_3Zr_2O_{12}$)
single crystal.

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Volume Crystals

Melt grown bulk $LaInO_3$ single crystals

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Heterojunctions between polar $LaInO_3$ and non-polar $BaSnO_3$ are a hot topic in current materials physics due to the formation of a high-mobility 2-dimensional electron gas (2DEG) with polarization doping and the perspective of field-effect transistor (FET) fabrication to exploit this phenomenon [1]. Since the availability of native $BaSnO_3$ substrates is still highly limited [2], the quest for lattice matched substrates for growing $BaSnO_3$ films led us to develop bulk $LaInO_3$ single crystals of a reasonable size and structural quality. Perovskite $LaInO_3$ has orthorhombic symmetry and crystallizes in the space group *Pnma*. Until now, bulk $LaInO_3$ crystals were demonstrated by the optical floating zone (OFZ) method only, that produced dark crystals of about 6 mm in diameter [3].

The ternary La-In-O system is thermally unstable at high temperatures and undergoes a substantial decomposition with In_2O and O_2 as the most volatile species. We measured the melting point (MP) of $LaInO_3$ at 1880°C ± 15 K. This temperature is high enough for significant loss of In-containing species that leads to a fast composition shift towards the La-rich side. At MP, the ratio of partial pressures of In_2O to LaO is at the level of six orders of magnitude even in a pure oxygen atmosphere. To minimize the decomposition during growth of bulk $LaInO_3$ crystals we utilized the Vertical Gradient Freeze (VGF) method with 40 or 60 mm diameter Ir crucibles that were heated up inductively.

The starting composition was incongruent with a general formula of $LaIn_{(1+x)}O_3$ with x = 0…0.1. The growth atmosphere consisted of argon containing 9…14 vol.% O_2, atmospheric pressure was used during growth. Both heating up and cooling down times were between 5 and 8 h. As starting materials, La_2O_3 and In_2O_3 powders (5N) were employed, which were separately dried, mixed together, pressed, and sintered prior use. Some of the crystals were doped with Ba^{2+} or Zn^{2+} (to potentially induce p-type conductivity), with Si^{4+} or Sn^{4+} (to potentially induce n-type conductivity), and with Ce^{3+} (aimed to achieve a new potential scintillator). Undoped and intentionally Ba-doped $LaInO_3$ as solidified in the Ir crucibles are shown in Figs. 1a and 1b, respectively. The solidified material typically consisted of several $LaInO_3$ single crystal grains with a volume of 0.5…2.5 cm³ that enabled wafer fabrication with a size up to 10x10 mm² (Fig. 1c) in all main orientations (100), (010), (001), and (110). Undoped, Ce-, Si-, and Sn-doped $LaInO_3$ crystals were yellow, while Ba-, and Zn-doped were red. The obtained $LaInO_3$ crystals and fabricated wafers are now being used as substrates for $BaSnO_3$ film growth by PLD and MBE.

Fig. 1
Crystallized $LaInO_3$ material within Ir crucibles: (a) undoped, and (b) Ba-doped; and (c) fabricated (110)-oriented wafers from an undoped crystal.

(a) (b) (c)

The obtained crystals were of single orthorhombic phase of $LaInO_3$ with the following lattice parameters at RT: a = 5.9380(5) Å, b = 8.2143(5) Å, and c = 5.7227(5) Å. The composition analysis of the crystals revealed near-stoichiometric composition with a small In deficiency. The full width at half maximum (FWHM) of the rocking curves of fabricated wafers were between 57 – 80 arcsec (Fig. 2a). The AFM wafer evaluation showed a root mean square (RMS) surface roughness below 2 nm for main wafer orientations. A good surface could be obtained after annealing at 600°C for 1 h in air with a significant improvement of the RMS roughness to 0.126 nm and a terrace formation (Fig. 2b). However, annealing at higher temperatures, in particular above 800°C, makes the surface rougher, deteriorating with annealing temperature and annealing time. Ba- and Ce-doped $LaInO_3$ wafers revealed a better surface stability at high temperatures as compared with undoped wafers.

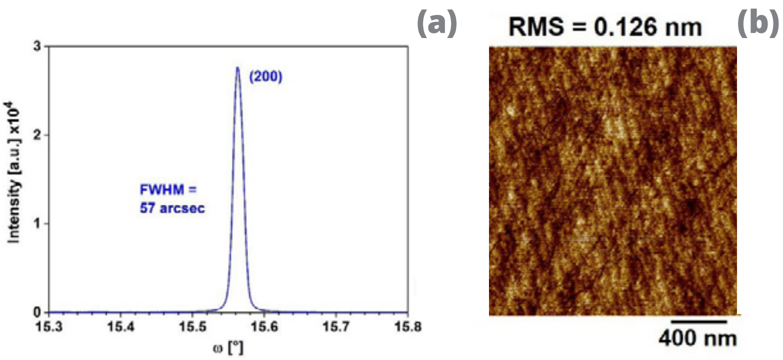

Fig. 2
(a) rocking curve; and (b) AFM image of a $LaInO_3$ wafer that was polished and annealed at 600°C for 1 h in air.

Further analysis of the thermal stability showed that the $LaInO_3$ crystals are substantially stable in oxidizing atmospheres up to 1200°C with no measurable mass loss and no phase transition, and up to about 500°C in reducing atmospheres.
All as-grown $LaInO_3$ single crystals, whether undoped or doped with Ba, Zn, Si, Sn, and Ce were electrically insulating. Also annealing in oxidizing and reducing condition did not change the electrical state of bulk crystals. We also determined the relative static dielectric constant, which is ε_r = 24.6 ± 1.1 along the [001] direction of $LaInO_3$.

Basing on measured absorption coefficients that are light polarization dependent, we extrapolated corresponding direct optical bandgaps (direct bandgap predicted by the theory) at room temperature 4.39 eV for the electric field vector E II [100] and [001], and 4.35 eV for E II [010], as shown in (Fig. 3a), in a good agreement with the theoretical predictions [4]. The crystals revealed, however, a weak absorption at about 2.8 eV (400 nm) that is clearly visible at two different sample thickness (Fig. 3b). According to DFT calculations [5], this weak absorption is caused by in-gap states that originate from oxygen vacancies.

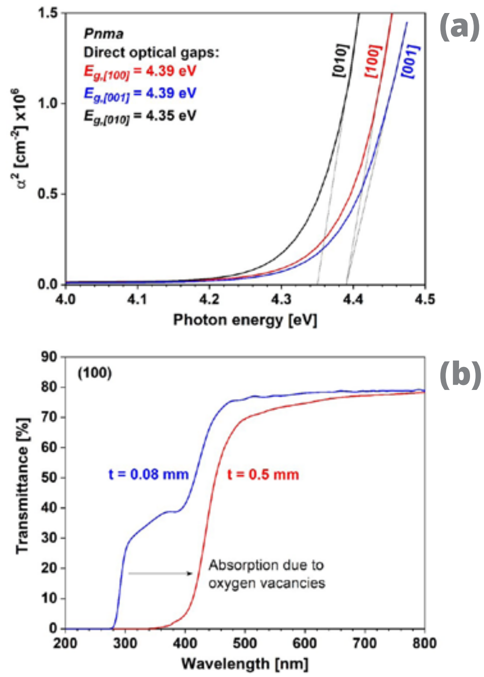

Fig. 3
(a) relation α^2 vs. photon energy for direct optical transitions of differently oriented $LaInO_3$ wafers; and
(b) transmittance spectra of $LaInO_3$ wafers of different thickness.

Acknowledgement

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Volume Crystals

Dislocation investigation in high purity Ge by white-beam X-ray topography and wet-chemical etching

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New generation radiation detectors with superior sensitivity require quality-tailored, high-purity germanium (HPGe) single crystals. These detectors are utilized in γ-ray detection and as well in the quest to detect very rare nuclear events, such as neutrinoless double-beta decay (0νßß) for better understanding the fundamentals of the universe. IKZ is an active member in the international LEGEND project [1] where 200 kg of HPGe detector crystals are needed to increase the discovery potential for 0νßß. High purity crystals for detector fabrication should contain incredibly low foreign impurities, i.e., one foreign atom out of 10^{13} host material atoms (about parts per trillion) and have a specific range of dislocations (10^2 to 10^4 cm^{-2}) that are homogeneously distributed. Hence, it is of crucial importance to investigate the structural defects and reliably determine their concentration within a crystal.

A low density of structural defects such as dislocations and voids ensure high lifetime of charge carriers leading to a better detector performance. However, completely dislocation-free Ge is unfavorable, since vacancies in such crystals dominate the defect landscape, resulting in vacancy-related complexes such as V_2H and vacancy clusters in the form of voids, rendering the material ineffective for detector applications. By controlling the temperature gradient during crystal growth, the distribution of dislocation density can be contained to a certain degree. In this study, [001] oriented, 2-inch diameter HPGe single crystals were grown by the Czochralski method under H_2 atmosphere. The Dash-necking procedure has been adopted to control the initial dislocation multiplication.

Synchrotron white-beam X-ray topography (WBXRT) is used to investigate the details of dislocation structures and also to detect the vacancy clusters (voids), manifesting in the form of localized tensile strain fields. We have performed WBXRT measurements in transmission (Tx) geometry (Fig.1) at Karlsruhe Research Accelerator (KARA) synchrotron in Karlsruhe Institute of Technology (KIT). For this investigation, (001)-oriented, double-side chemo-mechanically polished wafers with thicknesses of 700 and 350 µm were prepared from top and tail-parts, respectively, of the grown crystals. The topographs were recorded with Slavich VRP-M high-resolution photographic film and a 2-dimensional indirect detector with a pixel size of 2.5 µm. The total area of the samples investigated by WBXRT was of the order of cm^2 [2]. The horizontal measurement axis of the wafers was [110], and the samples were tilted around this axis by 14° and by 28°, to reach the desired 2-20 and 1-3-1 Bragg reflections, respectively.

The wafers prepared from top-part of the crystal show dislocation-free regions (Fig.2a). In those regions, micro-voids can be observed as round shaped features with a black–white contrast. We observed that voids occur only in dislocation-free parts of the crystal and do not show up wherein regions with homogeneous and moderate dislocation density. The voids originate from

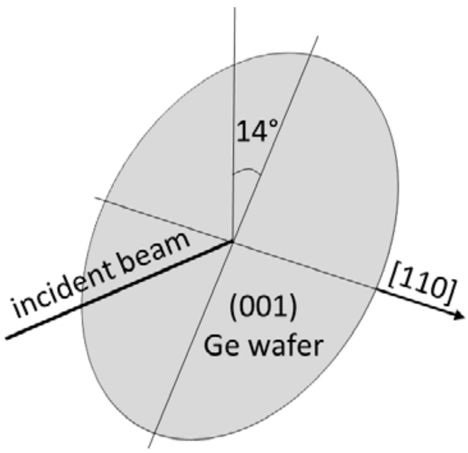

Fig.1
WBXRT measurement geometry for (001) Ge wafer. The 2-20 and 1-3-1 topographs were taken with [110] as a horizontal axis. Figure reprinted from Ref.2.

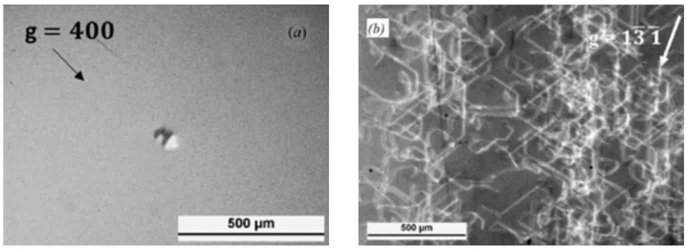

Fig. 2
Synchrotron Tx topographs of HPGe
(a) void observed in dislocation-free regions, in the top-part of the crystal. The voids are situated close to the exit surface of the beam and are only visible due to a dynamical diffraction phenomenon; (b) dislocation network with pseudo-hexagonal loops. No voids can be observed in this tail-part of the crystal, which has a moderate dislocation density of 3000 cm^{2}. Figures reprinted from Ref. 2, and from Ref. 3 (under Creative Commons Attribution 4.0 license) respectively.

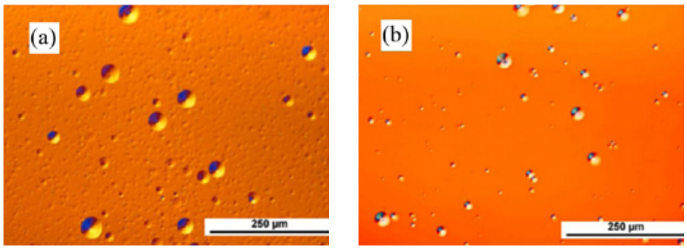

Fig. 3
Etching features observed using DIC microscopy on the samples cut from, (a) top-part of the crystal; (b) tail-part of the crystal. The large well-defined etch pits originate from dislocation cores. The dislocation-free wafer A also shows a differentiated etch figure (shallow pits) from the sample B with dislocations. Figures reprinted from Ref. 3 under Creative Commons Attribution 4.0 license.

clustering of vacancies during the growth process. The vacancy concentration at the melting point of Ge is of the order of 10^{14}–10^{15} cm^{-3}. This is several orders of magnitude larger than the concentrations of self-interstitials (10^{9} cm^{-3}) and impurities (<10^{12} cm^{-3}), and therefore, the vacancies are not completely annihilated during the crystal cooling process. So, in the case where there are no dislocations, the vacancies ultimately have to cluster as voids and will have deterimental effect on the detector performance. But, the presence of dislocations with edge character would allow the vacancies to be fixed around the dislocation lines, so-called dislocation decoration, and act as an effective sink for vacancies. The dislocation densities of the wafers were found to be below 1 cm^{-2} at the top-part of the crystal (Fig.2a), and is 3000 cm^{-2} for the tail-part (Fig.2b).

Since dislocations can act as the preferred etching sites, they could also be investigated by simple wet-chemical etching method. The etching was performed using a modified CP-4 etching solution. The etched wafers were investigated by differential interference contrast (DIC) microscopy and an etch pit density (EPD) analysis was conducted in order to infer the defect density and its uniformity throughout the crystal [3]. The large etch pits are composed of {111} facets (octahedral-shaped) with a rounded bottom (Fig.3). The average values of EPD calculated for the top-part of the crystal are high and are around 5000 cm^{-2} (Fig. 3a), and do not agree with WBXRT measurements. Almost dislocation-free samples show a high density of ''tiny'' shallow etch pits, which are distributed over the entire surface. One may say that these tiny pits, which represent small prismatic dislocation loops, would form due to other preferred etch sites arising from vacancy condensations (voids) or vacancy-associated complexes. Although the etching differs between the dislocation-free and the dislocation-containing parts of the crystal, the characteristic dark pits (octahedral) do not allow us to unambiguously distinguish the etching features related to voids and dislocations. For the dislocation-free HPGe samples, the chemical etching process conditions must further be altered and optimised to delineate the features. On the other hand, the EPD value for the tail-part of the crystal (Fig. 3b and 2b) from etching method matches well with the XRT-measured dislocation density value of 3000 cm^{-2}.

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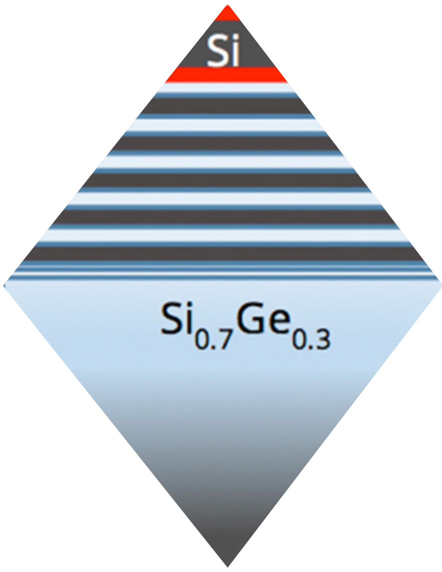

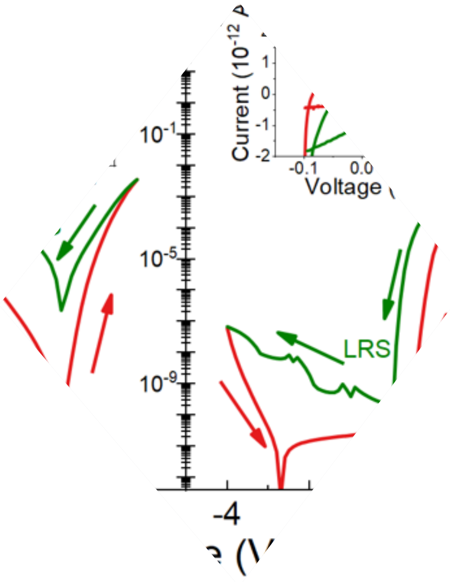

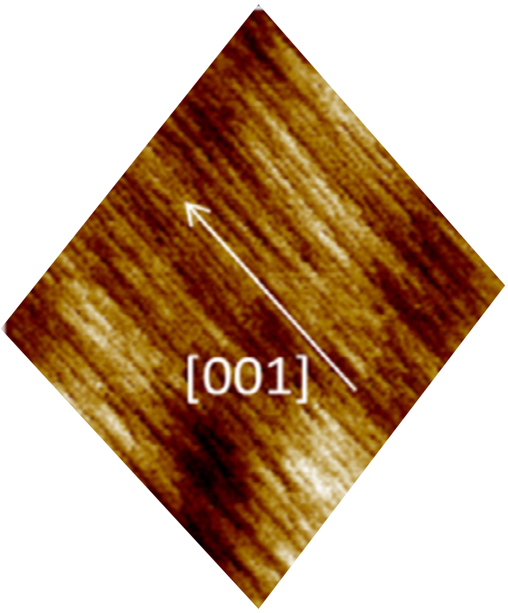

Nanostructures & Layers

CVD and MBE growth of strained Si layers for quantum computing devices

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The development of computing devices has reached a turning point. Moore's law comes to an end due to the physical limits of miniaturization. Quantum computing with its very different approach based on quantum mechanical principles is predicted to reach a new level of sophistication. In recent years different concepts evolved [1], realizing quantum bits (qubits) from physical systems like trapped ions, superconducting circuits or nitrogen vacancies in diamond. One of the most promising concepts is based on single electrons in semiconductors, since the system can be scaled up to very large numbers of qubits and also has the advantage that existing manufacturing technologies may be adapted.

Electron spin states in this system can be employed as qubits. The logic space formed by these quantum states is enormous, since they can also exist as superposition states. This is far beyond the "1" and "0" switching logic of common (classical) processors where a charge state formed by several electrons on a distinct place makes the difference between "on" or "off". Another prerequisite for quantum computing is that the states of the qubits have to be "entangled", that means they are directly correlated with each other. They behave like a tandem and measuring the state of one particle will directly determine the output of the other. Already a few double-qubits when having a high fidelity can open new worlds of computation. The preconditions for operation on the mK temperature level are: A strong energetic confinement in an environment that is free of magnetic noise and parasitic electrical charges. A tensile-strained, few nanometers thin Si layer sandwiched between SiGe layers with atomically sharp interfaces forms a quantum well for a two-dimensional electron gas and fulfills these requirements in every respect [2].

Such structures were epitaxially grown in our group by molecular beam epitaxy (MBE) in the framework of the Leibniz Competition project "SiGeQuant". A high-pure and highly enriched monoisotopic ^{28}Si source was used for this purpose. In this way, electrically active impurities and the nuclear magnetic noise of ^{29}Si can be avoided to a great extent.

The MBE growth is performed on a chemical vapor deposition (CVD) strain-released buffer (SRB) SiGe substrate [3] that was developed on a commercial Si(001) wafer at the Leibniz Institute for High Performance Microelectronics IHP. The seamless transfer of the SRB substrate from the CVD chamber in Frankfurt to the MBE chamber in Berlin was organized in close co-operation. After wet chemical surface cleaning of the SRB SiGe substrate a smooth surface with a roughness lower than 1 nm was obtained before starting the MBE growth of the ^{28}SiGe/^{28}Si/^{28}SiGe heterostructure. Both ^{28}Si and ^{nat}Ge were evaporated from solid state sources. Here, the ^{28}Si source whose isotopic purity is more than 99.99 % is provided by the Float-Zone Si group of the IKZ, who has long-standing expertise in preparing high-pure and highly-enriched ^{28}Si single crystals as were required in the former Avogadro project.

To characterize the structure and the purity of the strained ^{28}Si film, several characterization methods are involved. The appropriate structural properties of the layer stack have been revealed by transmission electron microscopy (TEM). One of the scanning transmission electron microscopy (STEM) images is shown in Fig. 1, where the interfaces of ^{28}SiGe and ^{28}Si are clearly indicated. Both isotopic and elemental impurity contents were measured by second ion mass spectroscopy (SIMS). The SIMS profile of mass 29 shows the low level of parasitic ^{29}Si atoms within the MBE layer (see Fig. 2). Compared to the CVD grown SRB SiGe substrate where natural Si with a fraction of 4.67 % ^{29}Si was applied, the ^{29}Si concentration dropped more than two magnitudes.

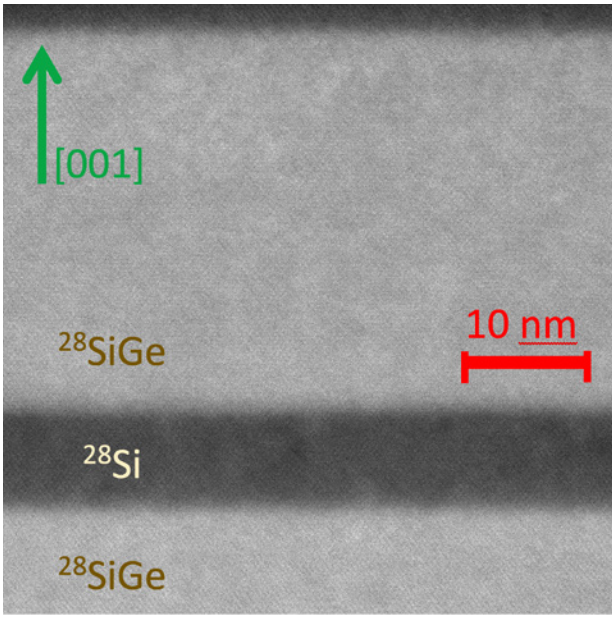

Fig. 1

STEM of ^{28}SiGe/^{28}Si/^{28}SiGe heterostructure:

The growth direction is [001] shown in the image with an arrow.

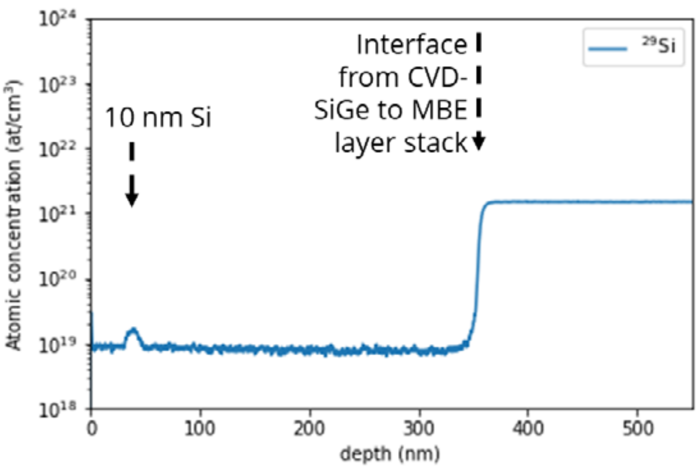

Fig. 2

SIMS plot of the ^{29}Si content within the MBE grown quantum structure: $^{28}Si_{0.7}Ge_{0.3}$ capping layer (left), tensile-strained ^{28}Si quantum well, $^{28}Si_{0.7}Ge_{0.3}$ base layer, and CVD grown nat$Si_{0.7}Ge_{0.3}$ strain-relaxed buffer (right).

The low ^{29}Si impurity level within the strained Si layer implies that the decoherence influence of nuclear spins on the electron spin should be very low in future devices. Furthermore, other characterization methods are also involved. The strain state has been investigated both by reciprocal space map (RSM) method with X-ray diffraction (XRD) and by μ-Raman mapping. RSM shows that on the one hand that the ^{28}SiGe layer grown by MBE matches well with the composition of SRB SiGe substrate and on the other hand that the thin ^{28}Si layer is fully strained. The μ-Raman mapping reveals that strain fluctuation of the ^{28}Si is below 0.2 %. The surface roughness was measured by scanning force microscopy (SFM), where it shows that the surface roughness of ^{28}SiGe/^{28}Si/^{28}SiGe is similar to the surface roughness of the SRB SiGe substrate and also below 1 nm.
Our ^{28}SiGe/^{28}Si/^{28}SiGe structures will be processed to qubit test devices by partners at the RWTH Aachen, the Institut für Quanteninformation (IQI) and the Institut für Halbleitertechnik (IHT).

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Epitaxial $SrTiO_3$ thin films grown by MOVPE for memristive devices

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Unstrained stoichiometric strontium titanate ($SrTiO_3$) is an ideal cubic perovskite oxide, which exhibits high permittivity and high resistivity. In recent years, especially $SrTiO_3$ thin films have gained increasing interest due to their resistive switching properties, rendering them a potential candidate for memristive devices with the vision to mimic human brain function in artificial intelligence networks. However, the underlying physical origin of the resistive switching mechanism is still unclear and a controversial discussion to date.

The most popular and accepted model is based on oxygen vacancies which are considered to form conductive filaments in an insulating material by the application of a bias and hence lead to a low restive state (LRS). By changing the direction of the electric field, filaments are ruptured resulting in a high resistive state (HRS). This processes of forming and rupturing hence are based on ion diffusion induced by an electric field. However, such a filament formation is expected to be orders of magnitude more decelerated compared to experimentally observed switching cycles.

Furthermore, with respect to application in resistive switching devices, the formation of filaments is highly undesired. They are formed stochastically distributed and are therefore expected to cause a large variance in switching parameters of a single memory cell during successive switching cycles and of different memory cells on the same chip. But also, other mechanisms are plausible to explain the observed bipolar resistive switching effect in $SrTiO_3$ thin films which are for instance based on Schottky barriers or charge (de)trapping effects.

In order to shed light on the switching mechanism, in the Leibniz competition project "Physics and control of defects in oxide films for adaptive electronics" $SrTiO_3$ thin films have been grown with highest possible structural perfection and investigated with different characterization techniques working on both microscopic and macroscopic scale. The facilities at IKZ provide ideal conditions for this project, as they offer besides advanced structural ("Electron microscopy" group) and electrical characterization techniques ("Physical characterization" group) also the ability and knowledge to grow $SrTiO_3$ thin films by metal-organic vapor phase epitaxy (MOVPE) in the section "Thin Oxide Film".

Since MOVPE takes place near the thermodynamic equilibrium and at high oxygen partial pressure, it facilitates the growth of stoichiometric as well as deliberately off-stoichiometric films with high structural perfection. Contrastively to the mostly employed PLD method, our liquid delivery spin MOVPE technique provides the precise and independent adjustment of the Sr, Ti, and O content in the films by controlling the respective precursor supply fluxes. Since epitaxial growth of $SrTiO_3$ by MOVPE has not been described in literature before, the first challenge to tackle was to develop an adequate process for stoichiometric, single-crystalline, "perfect" $SrTiO_3$ thin films homoepitaxially grown on $SrTiO_3$ substrates. This was successfully achieved by optimizing numerous growth parameters such as the substrate temperature, evaporation temperatures of the Sr and Ti precursors as well as their concentration ratio in the source liquids ($(Sr/Ti)_{liq}$).

To grow stoichiometric $SrTiO_3$ thin films, the most critical parameter is the $(Sr/Ti)_{liq}$ ratio, which was varied until the vertical lattice parameter of the film corresponds to the $SrTiO_3$ bulk value of 3.905 Å. This was achieved for $(Sr/Ti)_{liq}$ = 3.6 (see Fig. 1c). Scanning transmission electron microscopy high-angle annular dark-field (STEM)-HAADF images of this film show homogeneous intensity distribution and only faint contrast differences between film and substrate; no extended defects are visible (Fig. 2d).

Starting from stoichiometric $SrTiO_3$ films, we systematically decreased the Sr-to-Ti ratio in the gas phase which was achieved by varying $(Sr/Ti)_{liq}$. Evaluation of high-resolution x-ray diffraction (HRXRD) measurements exposes a pronounced shift of the film peak to the substrate peak (see Fig. 1a and with higher magnification in Fig. 1b), which corresponds to a strong increase of the vertical lattice parameter $d_{\perp}$ of the $SrTiO_3$ films with decreasing Sr/Ti ratio in the liquid supplies (see Fig. 1c). Reciprocal space maps and in-situ HRXRD measurements during heating in pure oxygen atmosphere up to 950°C further revealed that the deviation from bulk vertical lattice parameter can't be attributed to lattice strain relaxation or oxygen vacancies, but to a lattice expansion provided by the increased cation repulsion due to cation deficiency.

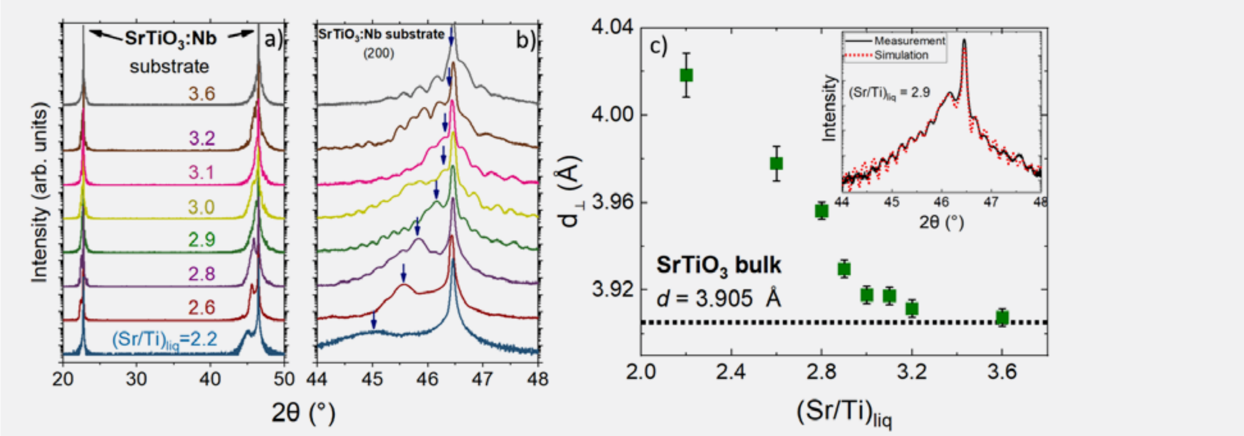

Fig. 1

HRXRD patterns (2θ/ω scan) of the $SrTiO_3$ thin films grown with varying $(Sr/Ti)_{liq}$ (a) in a wide 2θ range from 20° to 50° revealing the absence of parasitic phases, and (b) in the vicinity of the (200) substrate peak showing a systematic shift of the film peak with $(Sr/Ti)_{liq}$. (c) The evaluated vertical lattice parameter d⊥ as a function of $(Sr/Ti)_{liq}$. The inset shows exemplarily a simulated pattern with $(Sr/Ti)_{liq}$=2.9.

For films grown with $(Sr/Ti)_{liq}$ < 3.6, STEM investigations showed an inhomogeneous cloudy dark and bright intensity pattern (exemplary shown in Fig. 2c), which also have an overall darker contrast compared to the $SrTiO_3$ substrate. Since STEM-HAADF intensity is sensitive to atomic number Z, we concluded that here Sr deficiency related point defects are present to a large amount up to 20 %. Neither XRD nor TEM measurements indicated the occurrence of a foreign phase despite the observation of a strong Sr off-stoichiometry.

In order to investigate the influence of such a Sr deficiency on the electrical properties, current-voltage (IV) measurements were performed in a metal-oxide-semiconductor test structure consisting of a Niobium-doped $SrTiO_3$ substrate and Pt top contacts. To reveal the effect of off-stoichiometry, the IV curves of a stoichiometric film ($(Sr/Ti)_{liq}$ = 3.6) and of a $SrTiO_3$ with a pronounced off-stoichiometry ($(Sr/Ti)_{liq}$ = 3.2) are shown in Fig. 2b and a, respectively. The Sr-deficient thin films exhibit a distinctive intrinsic resistive switching behavior between the LRS and HRS (Fig. 2a), whereas for stoichiometric films, stable resistive switching could not be observed in the same voltage range (Fig. 2b).

The switching behavior for the off-stoichiometric films actually agrees well with the behavior of typically oxygen deficient PLD films. But there are some clear differences: Firstly, at 10 K – where ionic diffusion processes are strongly suppressed – the HRS in our MOVPE films is becoming more insulating, which cannot be explained by oxygen vacancy incorporation or diffusion. Furthermore, behavior in our case is not achieved by an abrupt switching but rather gradually introduced. Additionally, filaments could not be experimentally proven by in-situ STEM investigations in the applied voltage range. In sum, all these results imply that the underlaying mechanism here is not based on the formation of filaments. Careful evaluation of STEM data indicates a phenomenon based on Ti_{Sr} antisite defects as introduced by Klyukin et al. [1]. More details to the electric measurements and STEM results are given in Baki et al. [2].

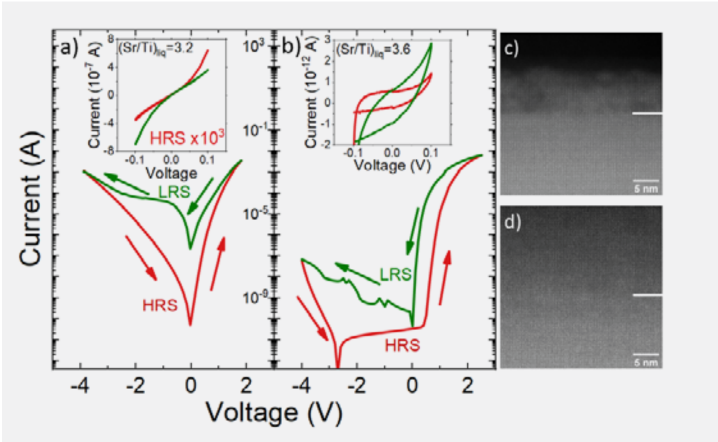

Fig. 2

IV measurements in the voltage range from -4V to 2V for $SrTiO_3$ samples with

(a) $(Sr/Ti)_{liq}$ = 3.2; (off-stoichiometric) and

(b) $(Sr/Ti)_{liq}$ = 3.6; (stoichiometric).

The corresponding STEM images are shown in (c) and (d). The interface between substrate a film is labeled by a short white line.

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β-Ga_2O_3 for highpower device applications

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Beta-type gallium oxide (β-Ga_2O_3) is a transparent semiconductor with a wide band gap of about 4.85 eV and very promising perspectives, especially in high-power device applications and solar-blind UV photodetectors. For high-power switching, β-Ga_2O_3 is forecasted to outperform the leading technology based on SiC and GaN due to a three times higher theoretically predicted electrical breakdown field. Therefore, β-Ga_2O_3 is attractive for future use in electric power grids, which will be based on much more efficient power conversion systems, thereby contributing to lowering the overall CO_2 production.

β-Ga_2O_3 transistors are based on a β-Ga_2O_3 substrate and an epitaxial β-Ga_2O_3 layer which acts as the electrical active part of the device. The device performance strongly depends on the quality of the epi-layer: a high crystalline layer quality and low defect densities are crucial to achieve excellent electrical properties.
At IKZ, the β-Ga_2O_3 bulk crystal is grown by the Czochralski method where the crystal is pulled out of the melt in the (010) direction. Parallel to the pulling direction wafers are prepared with the orientation (100) and (001). This wafering has been done externally at CrysTec GmbH in Berlin. In the past the (100) orientation has been selected since it is a cleavage plane and exhibits the lowest surface energy. (100) oriented wafers were prepared with an offcut angle of 6° towards [00-1] which results in a regular step-and-terrace morphology with a terrace length of about 5 nm. The step width of 5 nm was adjusted to the effective diffusion length of the Ga ad-atoms, thus leading to step-flow epitaxial growth mode.

Nevertheless, since the offcut is prepared by polishing thicker wafers, this procedure is highly material consuming. Therefore, instead of adapting the substrate offcut (and corresponding terrace length) to the effective diffusion length of the Ga ad-atoms, we focused rather on controlling their effective diffusion length. This required the following adaptation of the MOVPE growth parameters: First, we increased the chamber pressure to reduce the desorption of Ga atoms from the surface. Second, the increase of the chamber pressure in turn required an increase of the Ar push-gas. This will allow the material to reach the substrate surface although the thickness of the boundary layer will increase due to the higher chamber pressure. Finally, to provide more material on the surface, we also increased the Ga flux and with this the Ga/O ratio.

Oxygen reacts with Ga on the hot substrate surface during growth. Kinetic Monte Carlo (KMC) calculations show that a high oxygen amount decreases the diffusivity of the Ga atoms on the surface, due to their interactions [1]. By adjusting the Ga/O ratio the effective diffusion length of the Ga ad-atoms can be tuned and as a result we are able to control the growth mode.

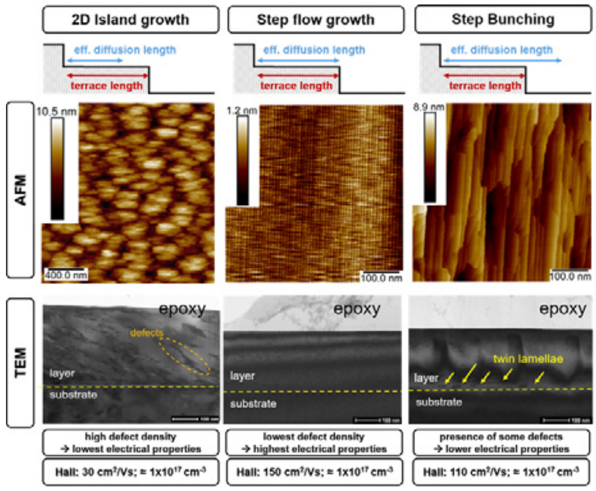

Fig. 1
Overview of the different growth modes and the corresponding effective diffusion lengths. AFM and TEM images show the morphological and structural properties, respectively. The electrical properties are shown representatively below the pictures.

Fig. 1 shows the influence of the effective diffusion length to the growth mode. The growth mode in turn strongly correlates with the morphological and structural quality and electrical properties of the epi-layer. In case of an effective diffusion length smaller than the terrace length the Ga ad-atoms will form 2D islands (see AFM picture upper left) since the Ga ad-atoms can't reach the step edges and will nucleate on the terraces.

Nanostructures & Layers

The layer will grow twinned on the substrate [2]. These twin lamellae act as defects, as visible in the TEM picture (lower left). Since a defect means a compensation center, this results in poor electrical properties. On the other hand, if the effective diffusion length is larger than the terrace length, step bunching occurs (AFM picture upper right) by superimposing of several steps. Also in this case a defected layer is the result (see TEM picture in the lower right).

These results clearly show that for films with a low defect density, it is crucial to adapt the effective diffusion length to the terrace length, where the Ga ad-atoms can reach the step edges and step-flow growth is obtained. Such layers grown in step-flow mode show smooth surfaces, low defect density and excellent electrical properties (AFM picture and TEM picture in the center). Therefore, we achieved epitaxial β-Ga_2O_3 layer with an electron Hall mobility of about 150 $cm^2\,Vs^{-1}$ at an electron concentration ~ 1.4 × 10^{17} cm^{-3} as shown in Fig. 2 [3]. This value of the electron mobility is the highest value reported so far for β-Ga_2O_3 thin films grown on offcut (100) β-Ga_2O_3 substrates and is in good agreement with the mobility values for β-Ga_2O_3 bulk crystals.

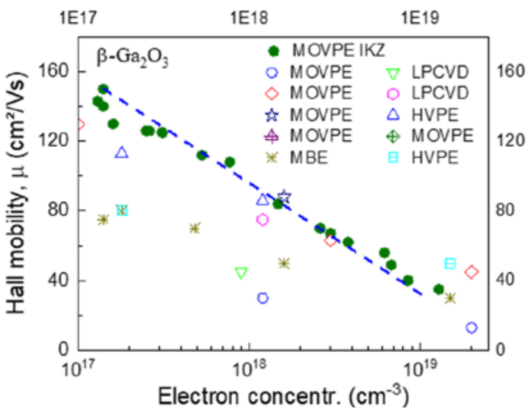

Fig. 2
The electron Hall mobility (green circles) of β-Ga_2O_3 films grown on (100) β-Ga_2O_3 substrate a function of electron concentration.

The successful control of the growth mode by adjusting the effective diffusion length allows to reduce of the necessary substrate miscut angle by maintaining the step-flow growth mode. A decrease of the miscut from 6° to 4° and even to 2° already means an increase of the terrace width from 5 nm to 8 nm and to 15 nm, respectively. Increasing the Ga/O ratio will also increase the effective diffusion length and step-flow growth mode can be achieved (see Fig. 3). This reduces the material consumption for wafer processing significantly

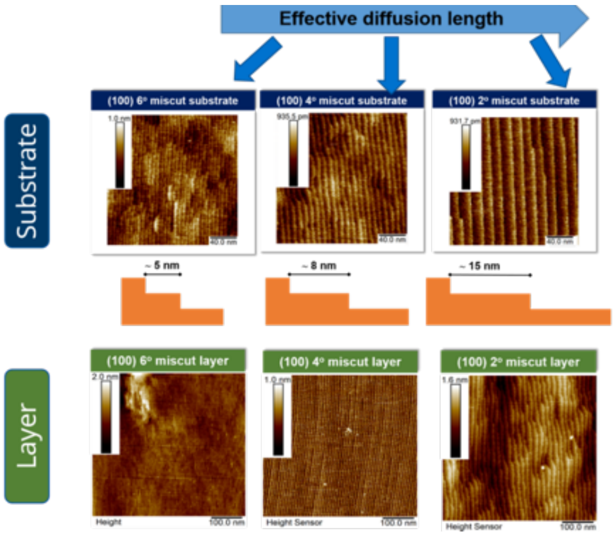

Fig. 3
AFM pictures of substrates with 6°, 4° and 2° offcut (upper line) and AFM pictures of the layer (lower line) on these substrates respectively.

This work was possible due to the good networking to the bulk oxide growth as well as structural and physical characterization groups in-house.

Acknowledgments

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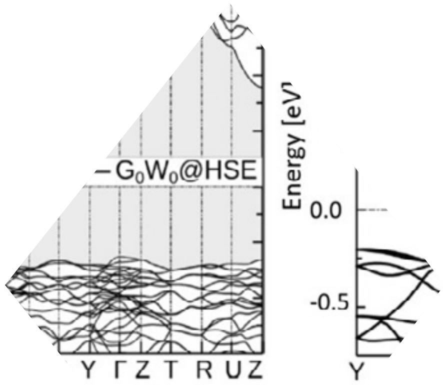

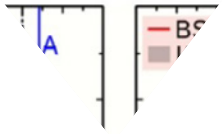

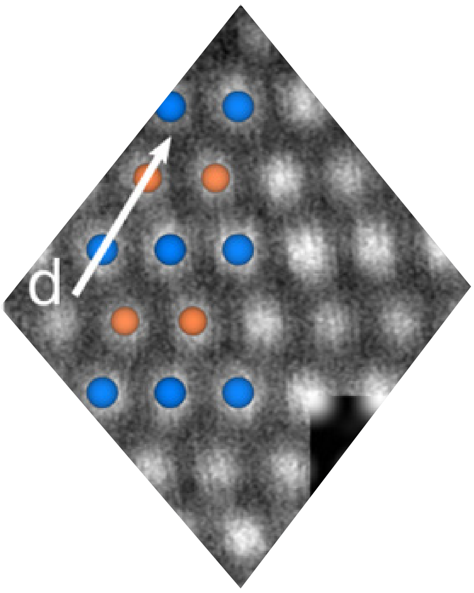

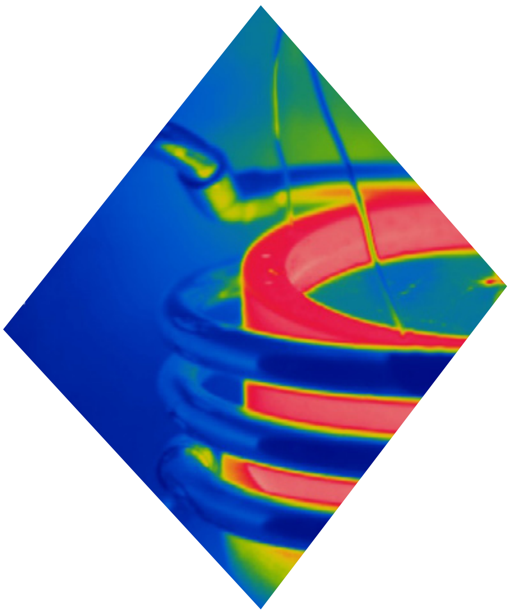

Materials Science

Band gap values from theory and experiment – A clarification exemplified for single-crystalline $LaInO_3$

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Lanthanum indate ($LaInO_3$) is a member of the material class of ternary oxides with perovskite structure on which the emerging field of oxide electronics with its promising multi-functionality is based. Presently, $LaInO_3$ is in the focus of investigations aimed on its usage in heterojunctions with barium stannate ($BaSnO_3$) which possesses the highest electron mobility observed so far among the semiconducting oxides. To understand the formation of the two-dimensional electron gas at the heterointerface, consistent data on the electronic band gaps of both materials from both theory and experiment are of primary interest. In a joint work we, theoreticians from the Humboldt University and experimentalists from IKZ, have performed a combined theoretical and experimental study of the electronic structure and the optical absorption edge of the orthorhombic perovskite $LaInO_3$.

If one wants to compare the theoretically calculated band gaps of crystalline solids with experimentally determined values, one has to consider several facts. The best known of these is that calculations based on density functional theory (DFT) in the context of the generalized gradient approximation (GGA) can underestimate the band gaps by up to a factor of 2, especially for wide-gap materials. This large error is due to the inclusion of an unrealistic electron self-interaction inherent in the method, which can be corrected by using hybrid functionals (HSE06). In the present work, we have gone a step further and determined the energies of independent quasiparticles (QP) within the G_0W_0 approximation based on the HSE06 calculations. Arrived at this level of bandgap calculation, however, two key interactions must still be considered to make a comparison with experimental values physically meaningful. The first issue is the nature of the experimental determination of the band gap. In most cases, optical measurements (e.g., as in our work, absorption spectra in the fundamental absorption region and spectroscopic ellipsometry) are performed.

Then the electron-hole interaction, i.e. the formation of excitons, plays an essential role. In the calculations, this can be adequately considered only in the framework of many-particle perturbation theory and is implemented by solving the Bethe-Salpeter equation (BSE). The attractive electron-hole interaction decreases the band gap compared to the value calculated for independent quasiparticles. We have performed corresponding calculations. The second interaction affecting the band gap is caused by the coupling of the electrons with the phonons in the crystal. Theoretical methods to account for the electron-phonon interaction are currently under development and could not yet be used in the present case. Thus, our calculations were based on the usual assumption of a rigid crystal lattice, i.e., the reduction of the bandgap with increasing temperature and the bandgap renormalization due to zero-point vibrations (ZPV) are not considered. However, we have been able to estimate the magnitude of this influence very well by temperature-dependent absorption measurements.

The main results of the present work are summarized in Figs. 1 and 2. Figure 1(a) shows the calculated electronic quasiparticle band structure (G_0W_0@HSE06), from which a fundamental band gap of direct nature at the Γ point of the Brillouin zone of 5.0 eV can be deduced. In Figure 1(b), the band structure in the immediate vicinity of the fundamental gap is considered in terms of possible optical transitions. For the conduction band minimum (CBM) and the upper six valence bands, the irreducible representations at the Γ point (A_{1g}, B_{2g}, ...) characterizing the symmetry are given, from which it can be seen which selection rules apply to electric dipole transitions in centrosymmetric $LaInO_3$. Accordingly, the transitions from the valence band maximum (VBM) and the following, energetically lower VB to the CBM are dipole forbidden (i.e. parity forbidden). This means that practically no optical absorption should take place across the fundamental band gap (transition "D" in Fig. 1(b)).

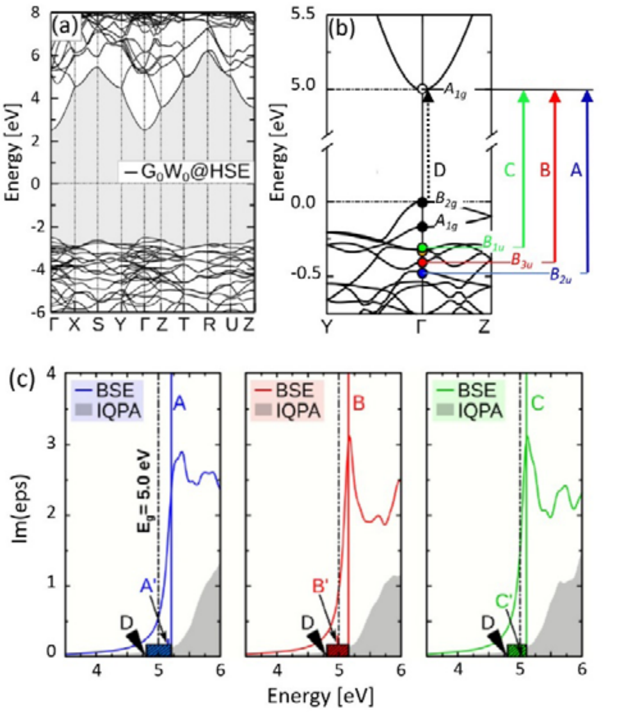

Fig. 1
(a) Electronic Band structure obtained from quasiparticle calculations based on the G_0W_0@HSE06 approximation.
(b) Symmetry analysis to predict the selection rules for electric dipole transitions at the Γ point of the Brillouin zone.
(c) Imaginary part of the dielectric function obtained by solving the Bethe-Salpeter equation (BSE) in comparison to quasiparticle calculations (IQPA).

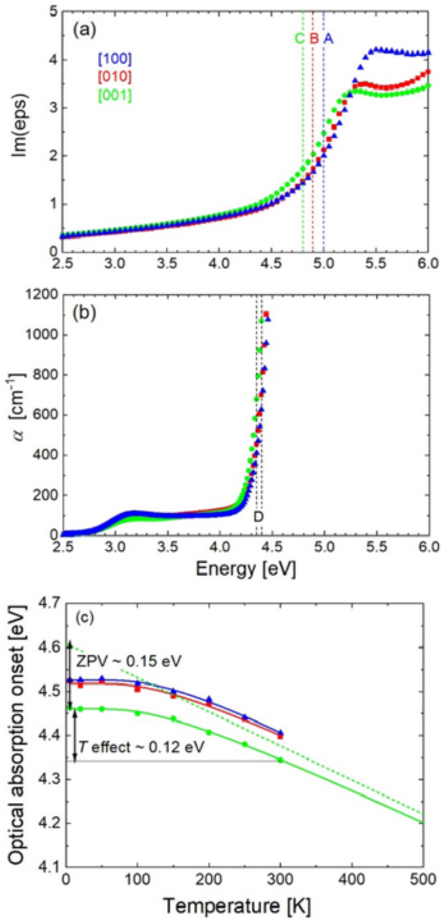

Fig. 2
(a) Imaginary part of the dielectric function measured by spectroscopic ellipsometry at room temperature (RT). (b) Spectral dependence of the absorption coefficient at RT near the fundamental band gap. (c) Temperature dependence of the optical absorption onset.

In contrast, the transitions ("C", "B", "A") from the deeper VBs (marked green, red, blue) are dipole-allowed and have polarization-dependent transition probabilities (optical anisotropy): "A" corresponds to the electric field vector E parallel to [100], "B" to E || [010], and "C" to E || [001]. This becomes quantitatively evident by the solution of the Bethe-Salpeter equation, the result of which is shown in Fig. 1(c). Moreover, comparison of the BSE results with those of the quasiparticle calculation provides that the optical energy gap (defined by transition "C") is redshifted by about 0.2 eV. This shift corresponds to the exciton binding energy; this is also approximately true for the other two transitions ("B" and "A").

For a comparison with the experiment, one has still to include the correction accounting for the electron-phonon interaction. For this purpose, we have measured the weak optical absorption ("dipole forbidden") near the fundamental energy gap as a function of temperature and fitted it with a single oscillator model as shown in Fig. 2(c). From this, one can estimate the influence of temperature and zero-point oscillations on the band gap. Thus, for the ellipsometry and absorption measurements shown in Figs. 2(a) and 2(b), respectively, which had been performed at room temperature, the theoretical transition energies must be reduced by 0.27 eV (0.12 eV temperature effect plus 0.15 eV ZPV) for comparison. Taking this correction into account, the experimentally determined positions for the transitions "A" to "D" plotted in dashed lines are in excellent agreement with the theoretical values.
Further details can be found in our publication referenced below.

This work was supported by the project BaStet (Leibniz Competition, No. K74/2017) that is embedded in the framework of GraFOx, a Leibniz ScienceCampus, partially funded by the Leibniz Association.

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The impact of order and cation coordination on the phase formation of $(In_{1-x}Ga_x)_2O_3$

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Solid-solutions of group-III sesquioxides (Al_2O_3, Ga_2O_3, and In_2O_3) show promise in designing new transparent *n*-type electrodes or active materials for optoelectronic applications because of the ability to tune the bandgap energies over large ranges (i.e., 3.6–7.5 eV) by varying the relative cation concentration. Group-III differ in their ground-state structures, which in addition offers the possibility of controlling the crystal structure by tuning the composition. Indeed, several current technologies such as optoelectronics, water splitting and piezoelectronics use structural modification by forming solid solutions as a route to widen potential applications.

To control the synthesis for advanced applications a fundamental understanding of the phase formation as a function of composition is required. Here we take $(In_xGa_{1-x})_2O_3$ as an example. Ga_2O_3 adopts the monoclinic (β) structure with space group C2/m with mixed four- and sixfold cation coordination, while In_2O_3 has a cubic bixbyite (c) structure with space group $Ia\bar{3}$ and sixfold cation coordination (Fig. 1). Additionally, these compounds display a rich phase space, with several polymorphs existing for both Ga_2O_3 and In_2O_3 that are somewhat higher in energy than the ground-state structures. In Ga_2O_3, the α ($R\bar{3}c$), γ ($FD\bar{3}m$), and orthorhombic κ ($Pna2_1$) phases have been reported in addition to the thermodynamically stable monoclinic β phase. In addition a hexagonal (h) $InGaO_3$ phase with space group $P6_3mmc$ has been observed, that contains fivefold and sixfold coordinated sites for the cations in equal amounts. Two recent works on $(In_xGa_{1-x})_2O_3$, based on density functional theory (DFT) calculations with limited configurational sampling [1, 2], are not consistent with each other and experimental work.

We therfore reevaluate the composition and temperature dependent phase diagram of $(In_xGa_{1-x})_2O_3$ heterostructural alloys through a joint computational and experimental investigation. We employ a computationally efficient protocol to search the vast configurational space of substitutional alloys using first-principles based cluster expansion models (CE) to understand the thermodynamics of these crystalline mixtures. We compare the computed thermodynamic phase diagram with experimental results from thin $(In_xGa_{1-x})_2O_3$ films grown by pulsed laser deposition (PLD) that are analyzed by high-resolution transmission electron microscopy to study the phase formation at the atomic scale.

Our experimental studies of heteroepitaxial $(In_xGa_{1-x})_2O_3$ films on c-sapphire substrates with a continuously varying indium content in the range $0 < x < 0.87$ and grown in the temperature range 640°C- 680° C by pulsed laser deposition yields the following main results [3]:

- For In contents up to $x = 0.5$, monoclinic single-phase films are observed.
- For In contents $0.55 < x < 0.7$, single-phase hexagonal $(In_xGa_{1-x})_2O_3$ is achieved.
- For In contents $0.7 < x < 0.91$, we find phase separation into the cubic ($x = 0.91$), monoclinic ($x = 0.5$) and hexagonal phase ($x = 0.7$).
- For In contents beyond $x > 0.91$, we find single phase material in the cubic bixbyite structure.
- The monoclinic and hexagonal lattices show a pronounced ordering on the cation sublattice (Fig. 2), with indium preferentially occupying the six-fold lattice sites, while gallium is mostly incorporated on the four- or five-fold lattice sites, in β- and h-$(In_xGa_{1x})_2O_3$, respectively.

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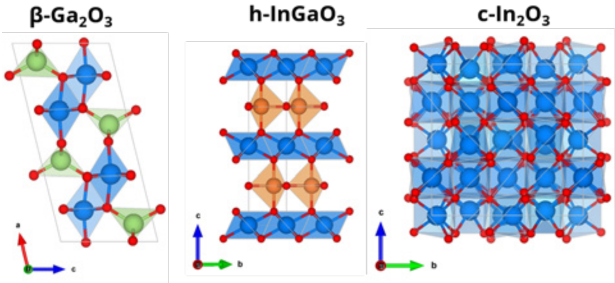

Fig. 1
Grond state lattice symmetries of Ga_2O_3, $GaInO_3$ and In_2O_3. The monoclinic, cubic bixbyite, and hexagonal phases have mixed four-/sixfold (green/blue), only sixfold, and mixed five- (orange)/ sixfold coordinated cation positions, respectively.

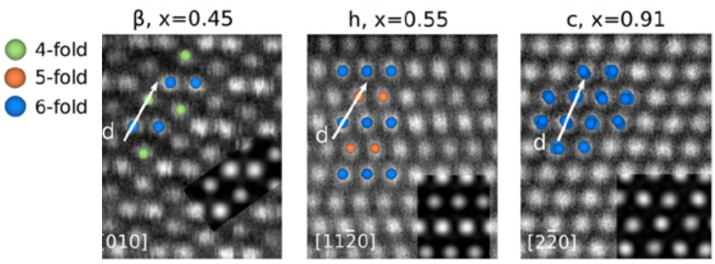

Fig. 2
Experimental high-magnification STEM-HAADF images (several images summed to enhance contrast) of monoclinic (ß) hexagonal (h) and cubic (c) $(In_xGa_{1-x})_2O_3$ alloys with overlay of the stick-and-ball models without oxygen atoms. The higher intensity of the fivefold and sixfold atomic columns, respectively, proves the preferential incorporation of the heavier indium to the sixfold lattice sites.

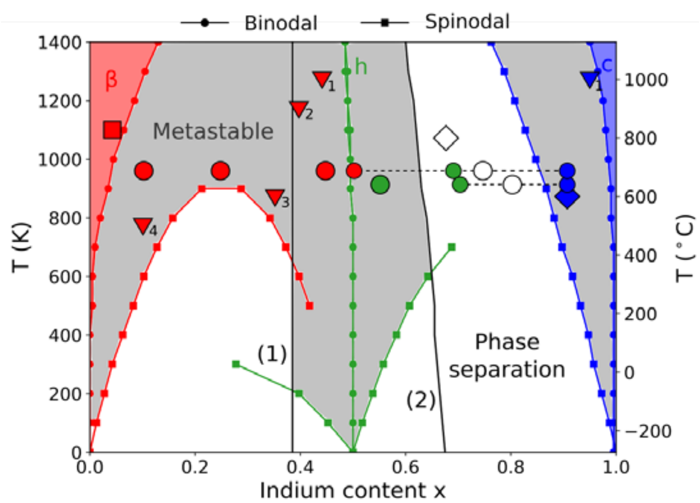

Fig. 3
Computed temperature dependent phase diagram for $(In_xGa_{1-x})_2O_3$ including binodal and spinodal lines for the monoclinic (blue), hexagonal (green), and cubic (orange) phases. Thermodynamic stable composition ranges are red blue, metastable ranges are grey, white area indicate phase separation. Experimentaldata points from PLD layers studied in this work (circles and diamonds) and from other synthesis methods found in literature (triangles) are added as symbols.

To calculate the phase diagram we start from the minimum energy configurations of the different phases at 0 K as identified by cluster expansion. The free energies at elevated temperatures are calculated by adding the configurational entropy. Since strong ordering on the cation sublattice is observed for the monoclinic and the hexagonal phase, even at relevant growth temperature, we modify the general assumption of ideal mixing in solid solutions and consider only coordination-specific sites. From the convex hull and curvature of the free energy curves we construct the full temperature dependent equilibrium phase diagram of $(In_xGa_{1-x})_2O_3$.

The accommodation of indium in the preferred sixfold environment leads to low mixing enthalpies in the composition range $0 < x < 0.5$ for β-$(In_xGa_{1-x})_2O_3$ and a remarkable stability for h-$(In_xGa_{1-x})_2O_3$ close to $x = 0.5$. This leads to a large metastable window in the gallium rich regime of the phase diagram for both phases (Fig.3). Experimentally we confirm miscibility in the monoclinic phase up to $x < 0.5$ as well as in the hexagonal phase at intermediate compositions up to $x = 0.7$. On the indium rich side of the phase diagram, a miscibility gap opens up to high temperatures, which is confirmed by experiment. The cubic phase, which has only one type of coordination site, is stable for $x > 0.9$ for growth temperatures around T = 1000 K, which fits well to the predicted metastable limit. In view of applications, the achievement of metastable compounds far outside the predicted thermodynamic equilibrium solubility limits is very promising and in excellent agreement with experimental findings by other authors (see [3] and references therein).

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New tools for modeling of crystal growth processes

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The new research group *Model experiments* funded by the Starting Grant NEMOCRYS from the European Research Council was established at the IKZ in 2020 [1]. Our goal is to investigate complex multiphysical phenomena in crystal growth processes on a macroscopic scale with a complementary use of dedicated model experiments and numerical simulation. In the first project year we focused on building an experimental platform (Test-CZ) and investigated heat transfer and electromagnetic aspects in the Czochralski (CZ) crystal growth process. A vacuum furnace at the IKZ was repurposed to resemble a typical CZ geometry as shown in Fig. 1, with inductive (IND) and resistive (RES) heaters and different outer crucible diameters (120 or 70 mm). The experimental setup includes comprehensive equipment for in-situ measurements:

- Thermocouples, resistance thermometers, and contactless pyrometers of various types to measure temperature in the crucible, melt, air, etc., as well as sensors for heat flux measurement through the insulation
- Optical cameras for process observation as well as an infrared camera for visualization of temperature gradients on the crucible surface, insulation, etc.
- Sensors for measurements of current and magnetic field of the inductors/heaters

In addition, dedicated calibration routines were developed for many sensors, and a flexible system for automatic data acquisition was set up in *Python* programming language.

In the Test-CZ setup we use model materials such as Sn and $NaNO_3$ to capture and analyze the relevant physical phenomena in CZ growth of materials such as Si and Ga_2O_3. Sn with a relatively low melting point of 232°C is easy to handle and has been already used in the past in CZ growth experiments [2]. In our first studies, Sn crystals were grown under various conditions (pull rate, crystal rotation, melt temperature, gas atmosphere, heating concept) and the resulting crystal diameter was evaluated. Together with detailed in-situ data these results were applied to validate numerical models (see below) but also to improve the physical understanding of the CZ growth process. What is the highest achievable growth rate for a given crystal diameter? How does the energy efficiency compare between induction and resistance heating? Which in-situ measurements could be applied for novel process control algorithms? These are just a few questions where these experiments allow for detailed "in-situ" insights. In future we will consider other model materials and investigate further physical phenomena such as flows in melt and gas phases using in-situ observations.

Numerical modeling is widely applied in crystal growth, but the underlying experimental data for model validation is scarce at best. Furthermore, commercial, black-box-type software with limited insight into the underlying numerical techniques has been applied in many cases. To address these issues, in the NEMOCRYS project we started the development of an open source platform for crystal growth simulation – *openCGS*, that is based on *Python* and allows for flexible coupling between pre-processors (e.g. *Gmsh*), solvers (e.g. *Elmer*, *OpenFOAM*, *FEniCS*), coupling libraries (e.g. *preCICE, EOF*), and post-processors (e.g. *ParaView*) as well as automated large-scale parameter studies. A new model for CZ growth based on *Elmer* [3] was implemented according to the following strategy (see also [4]):

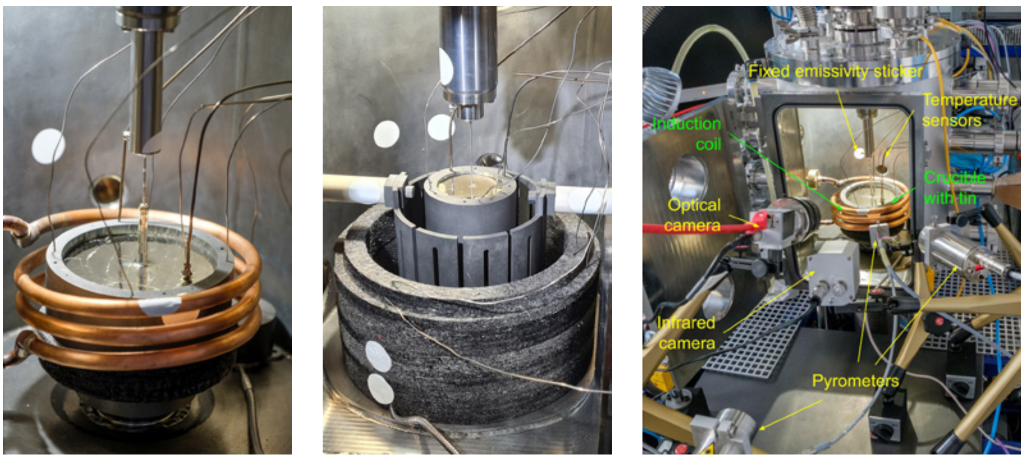

Fig. 1 Setup for CZ growth with inductive (left & right; IND/120 mm) and resistive (middle; RES/70 mm) heating showing the growing Sn crystals as well as measurement devices.

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- Verification of modules for heat conduction/radiation and electromagnetic heating in Elmer using analytical solutions
- Large-scale sensitivity analysis to identify the most important modeling and numerical parameters
- Validation of specific modeling assumptions (e.g. effective inductor current, effective heat transfer coefficient to account for gas cooling) using specific in-situ measurements
- Comparison of experiments and simulations (e.g. with respect to resulting crystal diameter) to evaluate the overall predictive capability of the model and provide detailed physical insight

To incorporate *Elmer* models in the *openCGS* platform efficiently, a new Python package *pyelmer* was developed and published with an open source license [5].

A study for the CZ growth of Sn with inductive heating is shown in Fig. 2. Verification showed an agreement with analytical solutions better than 5%. In the sensitivity analysis, the emissivities of furnace parts such as graphite crucible and steel vessel as well the convective cooling of the crucible were identified as key model parameters influencing the power balance of the furnace. To validate the global thermal model, the effective inductor current was determined from temperature measurements in vacuum (excluding convective heat transfer), while the effective heat transfer coefficient followed from the same experiment under air. The resulting model was used for a parameter study with various pull rates and melt temperatures, see Fig. 2 (right). A first comparison with experimental data indicates similar trends for the crystal diameter. A more detailed analysis will be performed in the future. The thermal model is currently being extended to include transient crystal motion and 3D furnace geometry.

In conclusion, several new tools have been established at IKZ for multi-physical crystal growth modeling: model experiments as a tool for physical insight, in-situ measurement equipment as a tool to obtain validation data for simulations, new numerical models as a tool to understand and optimize various crystal growth processes. These tools will be developed further to include more physical phenomena and other crystal growth processes such as the floating zone method.

Acknowledgements

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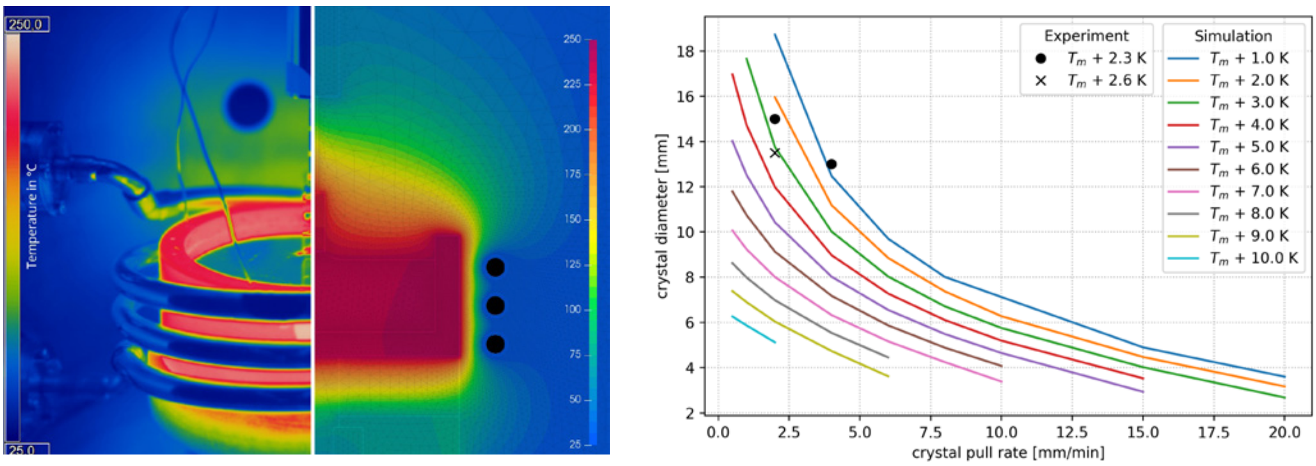
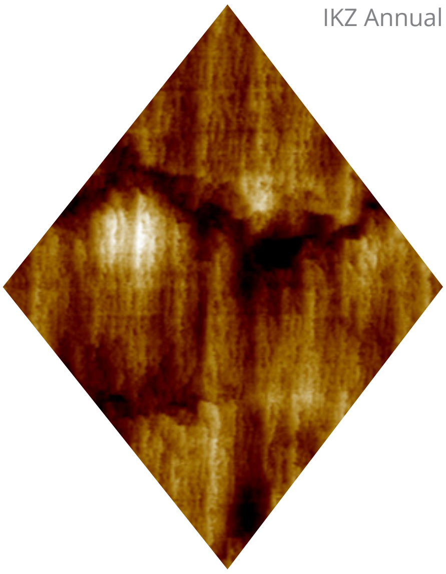
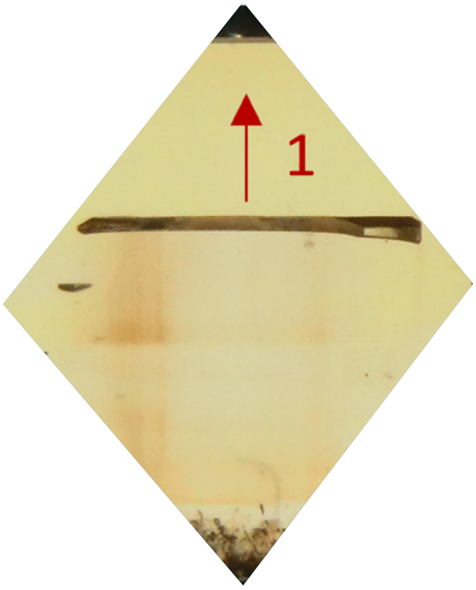
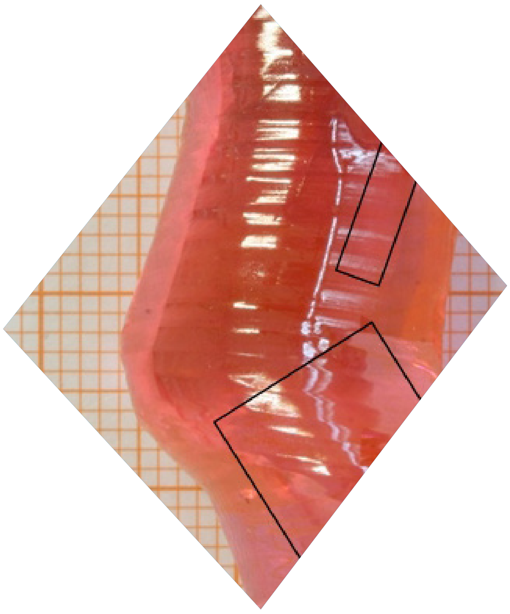
Fig. 2
Simulation of CZ growth of Sn crystals using openCGS/Elmer: temperature field in the simulation compared to an infrared image (left; setup IND/120 mm); crystal diameter vs. pull rate for various melt temperatures in simulations and experiments (right; setup IND/70 mm).









Application Science

Dislocation free bulk aluminum nitride crystals by sublimation growth – a XRT analysis

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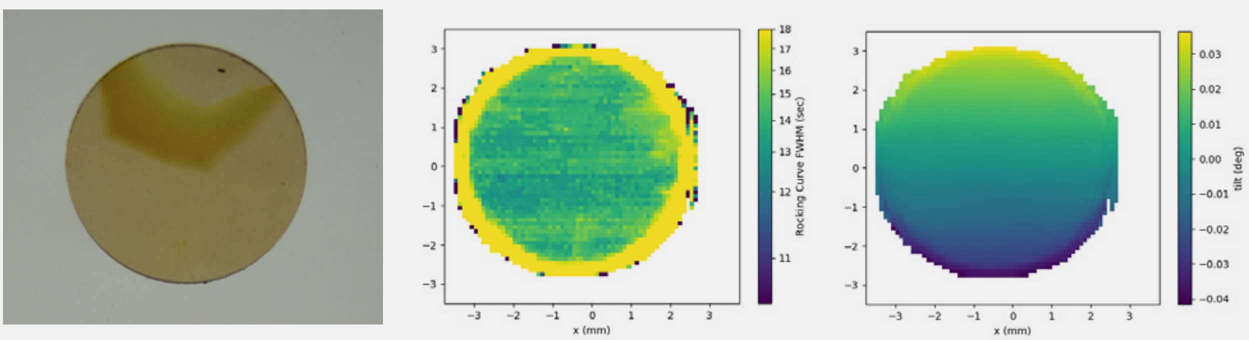
Aluminum nitride (AlN) is a promising substrate material for the fabrication of deep UV light emitting diodes (LED) [1], laser diodes (LD) and high power/high frequency electronic devices. Together with partners of the joint projects "AlN Substrate" und "AlN-230nm" funded by the Federal Ministry of Education and Research BMBF in the framework of the consortium "Advanced UV for Life", IKZ is presently developing AlN substrates for deep UV LEDs that can be used, among other things, for disinfecting water and various disinfection applications in the medical field.

A key element for the growth of bulk AlN crystals with low defect density is the proper fixation of seeds on a refractory metal seed holder stable at process temperatures higher than 2000 °C. This will avoid the formation of moving voids at the seed backside and subsequent defect formation. Although seeds from spontaneously nucleated crystallites defined geometry and high crystalline quality (EPD < 10^4 cm^{-2}) are available at IKZ, no lower dislocation densities could be achieved as the dislocations are typically transferred to the bulk volume during growth in c-direction [2]. Recently, we were able to demonstrate growth without dislocation generation along the c-axis and growth of dislocation free areas outside the original seed diameter by lateral growth at the crystal mantle, as evidenced by X-ray topography measurements.

Seeds with defined geometry and homogeneously low defect density are produced at IKZ by the spontaneous nucleation of crystals, subsequent preparation of round discs with a diameter up to 10 mm and chemo-mechanical polishing of the surfaces. Optical transmission images of a typical seed (Fig. 1, left) reveal two areas with different color impressions which are separated by lines forming an angle of 120° to each other. It can therefore be assumed that the areas grew in different crystal directions and therefore with different dopant incorporation – this is typical for crystals from a process without seed. Mapping of local rocking curve 0006 full-widths at half maximum (Fig. 1, center) shows that the crystalline quality is very good (FWHM < 18 arcsec), apart from a narrow edge region, and varies little locally. Mapping of the deviation of the crystal orientation normalized to the center position (Fig. 1, right) shows that the seeds have a global radius of curvature of approx. 6 m. As no local discontinuities of the orientation are present, we assume that no grain boundaries or mosaicity structures are present.

Fig. 1
AlN seed with D = 6 mm in transmitted light (left) with corresponding full-area measurements of the width of the (0006) rocking curves (center) and the deviation from the crystal orientation normalized to the wafer center in y-direction (right).



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In sublimation growth of AlN crystals, seeds are generally placed hanging above the AlN source, and therefore need to be fixed to prevent them from falling. This can be realized by placing the seed on an aperture made of a refractory metal and with inner diameter smaller than the seed diameter, or by gluing it on a seed holder made of a refractory metal and placing the seed holder on the crucible rim. The first method has the disadvantage that there is an initial loss of diameter, while with the second method there is a risk of thin cavities forming on the back of the seed during fixation, which coalesce during the growth process, migrate along the temperature gradient in growth direction and generate defects (Fig. 2). Experiments at IKZ have shown that a proper seed fixation by gluing can be realized using refractory metal foils and catalysts at defined temperatures > 1000°C; the latter aid in local liquid phase formation at the interfaces between the foil and the seed backside or seed holder front side.

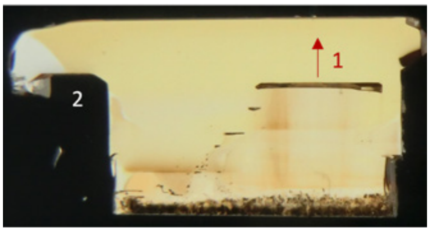

Fig. 2
Axial cut through a crystal grown on a fixed seed with voids that originated at the seed/seed holder interface and subsequently moved in c-direction (1) along the temperature gradient through the crystal. Strong lateral growth (2) occurs over polycrystalline growth next to the seed rim not visible in the picture.

AlN crystals were grown on seeds with 5 mm diameter and a dislocation density of approx. 10^4 cm^{-2} in a process developed at IKZ, with optimized seed-fixation technology and a well-adapted temperature field at the seed rim. Results are analyzed using transmission X-ray topography (XRT) imaging. A first XRT-image (Fig. 3, middle) with g = (0002) leading to extinction of a-type dislocation contrast shows that the sample does not contain dislocations with c- or c+a-type Burgers vectors. A second XRT-image (Fig. 3, right) with g = (1-100) shows an a-type dislocation density < 10^4 cm^{-2} comparable to the seed dislocation density (1) which attests our seeding technology - almost no additional dislocations are generated at the interface (2). Additionally, the complete absence of dislocations in the expansion region grown laterally exterior to the seed diameter (3) shows that dislocation reduction during subsequent seeding with diameter expansion is possible. Presumably, the dislocations propagating along the c-direction do not move or multiply in lateral directions. As a consequence, large dislocation free areas form during diameter expansion.

Acknowledgements

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The authors would like to thank Merve Pinar Kabukcuoglu from the Laboratory for Applications of Synchrotron Radiation (LAS) at KIT for the white beam images.

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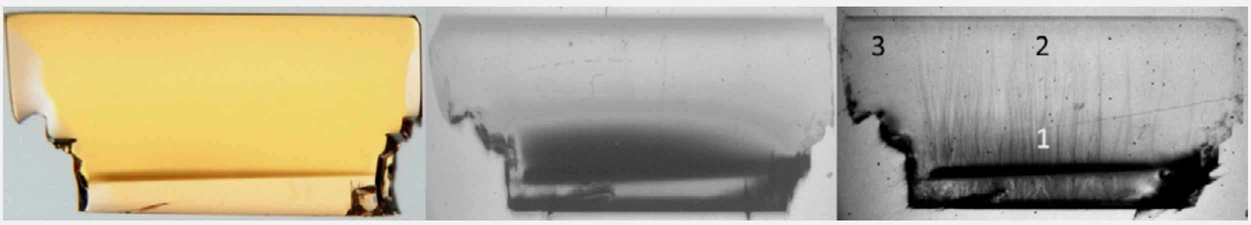
Fig. 3
Axial cut through AlN-crystal grown on a seed with 6 mm diameter in c-direction in transmission (left) and imaged with XRT using g = (0002) and g = (1-101) conditions and therefore showing only c-type (middle) and additional a-type (right) dislocations.



Application Science

Gallium oxide (010)-substrates for future power electronics – wafering challenges

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Crystalline gallium oxide is a promising substrate material for the production of next-generation power electronics devices [1, 2]. So far, gallium oxide crystals grown at the IKZ using the Czochralski process (CZ) have been used exclusively to produce substrates with (100) and (001) orientations, which can be cleaved along these easy cleavage planes and then polished also with off-orientation. However, since CZ-Ga_2O_3 crystals grow along the (010) direction and have a slightly elliptical shape, 2" diameter substrates can be efficiently prepared from crystals parallel to the (010) plane only. To evaluate the suitability of (010) substrates for epitaxy and device fabrication, crystals with a diameter of 20 mm were grown at the IKZ, processed into 5x5 mm² (010) substrates and successfully overgrown with gallium oxide epitaxial layers using MOCVD. The main challenge was to cut the crystals perpendicular to the cleavage planes without cracks and to polish them without chipping.

The IKZ has many years of experience in growing Ga_2O_3 single crystals using the Czochralski method [3] and in producing homoepitaxial layers [4], in particular on Mg-doped (100)-oriented Ga_2O_3 substrates with a defined off-orientation, which are usually produced from IKZ crystals by the industrial partner CrysTec GmbH. For these substrates, epitaxial growth conditions yielding step flow have been developed at the IKZ and, among other things, layers with a mobility of 153 cm^{-2} Vs^{-1} at a charge carrier concentration of 1.4 x 10^{17} cm^{-3} were demonstrated, see the report on Ga_2O_3 in the section "Nanostructures and Layers".
Fig. 1 schematically shows the preparation of 2" substrates from a typical CZ-grown crystal with a slightly elliptical shape and a minimum diameter of 2". Wafers with (010) orientation can be prepared with comparatively low material loss, but only a few wafers with (100) orientation. The preparation of (010) substrates therefore seems to be more economical at first glance. Anyway, decisive for the choice of substrate orientation is not only the substrate price but also whether high-quality epitaxial layers can be produced on the substrates or what device performance can be achieved.

Here, too, the race is still open. Step flow has already been demonstrated for epitaxial layers grown on substrates with (100) orientation, but although layers grown on (010)-substrates typically show no step flow but a facetted surface, also good layer properties can be realised on them [5].

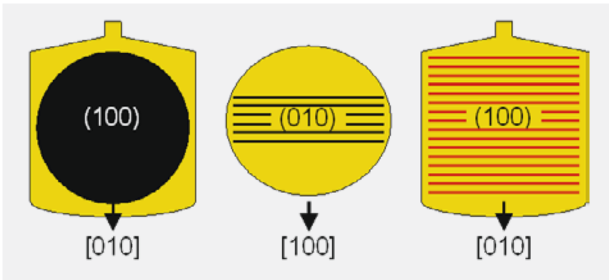

Fig. 1
Schematic illustration of the preparation of 2" substrates from CZ-Ga_2O_3 crystals with diameters > 50.8 mm in (100)-direction (left and centre; black circle and lines) and (010)-direction (right; red lines).

For the production of (010) substrates at IKZ, Mg-doped crystals with a diameter of approx. 20 mm and a length of approx. 50 mm grown in the (010) direction by the CZ-method at IKZ were used.
Due to the easy cleavage of the material gallium oxide along the (100) and (001) planes, cracks easily occur along the cleavage planes when cutting the crystals parallel to the (010) plane using standard processes (Fig. 2a and could only be avoided by embedding the crystals and using a special sawing technology (Fig. 2d). As the substrates tend to form chipping marks at the edges during polishing (Fig. 2b), they were protected by an embedding technology developed at the IKZ. This way, substrates with 5 mm and 10 mm edge length could be produced without edge chipping (Fig. 2e). Finally, material-specific chemical mechanical polishing processes were developed and optimized at the IKZ to produce surfaces without micro-scratches (Fig. 2f).

Application Science

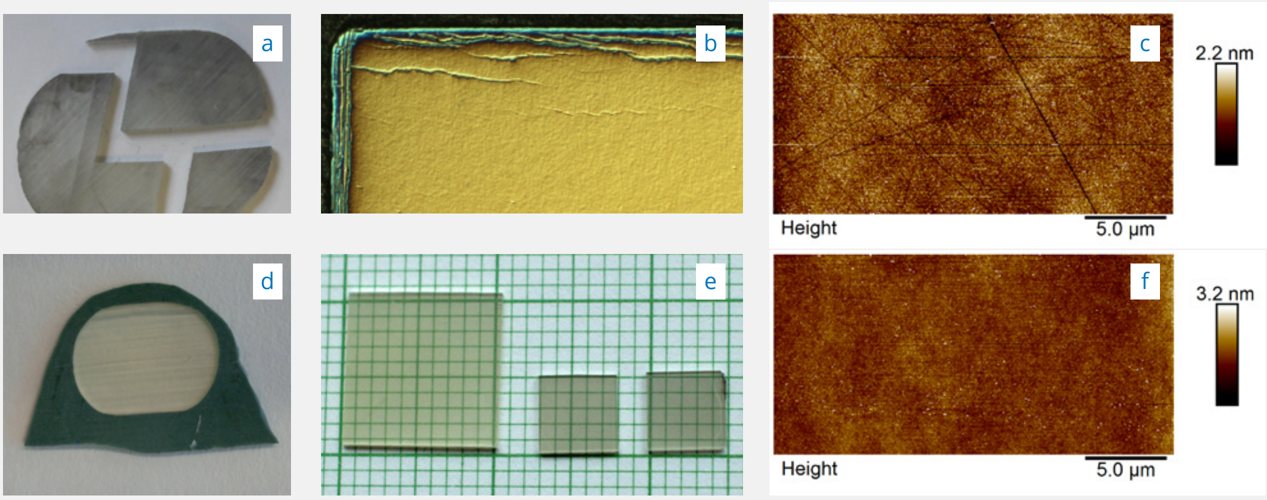

Fig. 2: Cut (a, d) and polished (b, e) Ga_2O_3-(010) substrates; AFM-pictures of CMP-surfaces with (c) and without (f) micro-scratches.

The gallium oxide substrates with on-axis (010) orientation were homoepitaxially overgrown at the IKZ with approx. 300 nm thick gallium oxide layers using MOCVD and standard process conditions at a growth rate of approx. 250 nm/h. The epilayer surface (Fig. 3) shows a facetted morphology with the appearance of elongated features oriented along the 001-direction which is well known and comparable to surfaces obtained at the IKZ and other research groups on commercially available (010)-substrates from Tamura Inc. [5].

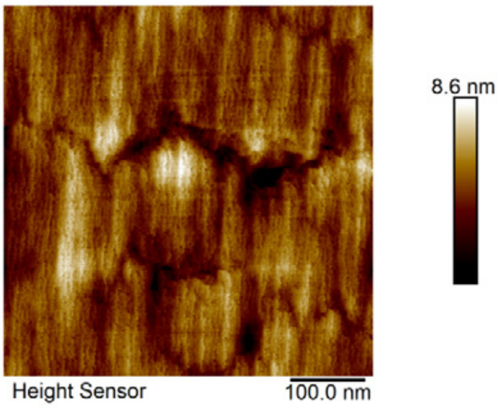

Fig. 3
AFM pictures of epitaxially grown Ga_2O_3-layers by MOCVD at IKZ on (010)-substrates from IKZ showing the for the (010) orientation typical facetted surface. The morhpology has a RMS value of 1.02 nm. Measurements of the elctrical properties by Hall showing a mobility of the layer of 100 cm^2/Vs at a carrier concentration of $7x10^{17}cm^{-3}$.

The properties of the grown layers will now be investigated in detail, and machining and epitaxy processes will be subsequently optimised or adjusted to (010)-substrates. In addition, the influence of the substrate misorientation on the layer properties will be evaluated.

Acknowledgements

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Application Science

Czochralski growth of mixed sesquioxide laser crystals

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Rare-earth sesquioxide crystals [1] are highly demanded for lasers and functional thin film growth. In particular the optically inactive members of these group, lutetia (Lu_2O_3), scandia (Sc_2O_3) and yttria (Y_2O_3) find many applications. They are excellent host materials for infrared lasers based on rare-earth doping ions and their large cubic lattice parameters make them highly suitable substrates for epitaxial thin film growth.

Unfortunately, these materials possess melting points well in excess of 2400 °C. Such temperatures are significantly above the highest temperatures on the order of 2200 °C possible during the Czochralski-growth of crystals from standard iridium crucibles. Therefore, in the past many different growth approaches utilizing expensive and sensitive rhenium-crucibles or crucible free techniques such as the optical floating zone method have been applied. However, none of these led to the development of a commercially applicable growth technology for cubic rare earth sesquioxide crystals.

In a collaboration between the Center for Laser Materials (ZLM) and the oxide crystal growth group at IKZ we re-investigated the phase diagrams of the ternary system Lu_2O_3-Sc_2O_3-Y_2O_3. In the largest range of compositions, these materials form cubic solid solutions according to $(Lu_xSc_yY_z)_2O_3$ with x+y+z = 1. These mixed sesquioxide crystals possess a disordered crystal structure, which features inhomogeneous broadening of the emission lines. The latter is a highly interesting feature for the generation of ultrashort laser pulses. Moreover, by compositional tuning the cubic lattice parameter can be adjusted for lattice matched thin-film substrates.

During these investigations, performed in a high temperature differential thermal analysis (DTA) setup utilizing tungsten-rhenium thermocouples, we found the melting points of the mixed crystals to be significantly reduced compared to the pure sesquioxides. In the binary system Sc_2O_3-Y_2O_3 we experimentally confirmed liquidus temperatures as low as 2100 °C, which were even further reduced to 2050 °C when doped with laser active trivalent erbium ions. These liquidus temperatures are 100 °C below previously reported values measured by pyrometric techniques. In a wide range of compositions of the refined ternary system shown in Fig. 1 the liquidus temperatures are below 2200 °C and thus in the range accessible for the standard Czochralski growth method from iridium crucibles.

The lattice constants for mixed sesquioxides with growth temperatures below 2200 °C can be tuned between 10.1 Å and 10.4 Å.

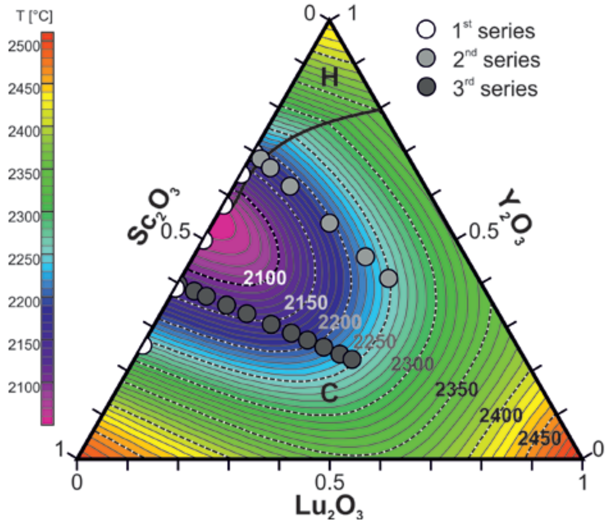

Fig. 1
Refined ternary phase diagram Sc_2O_3-Y_2O_3-Lu_2O_3. White, grey and dark grey dots indicate the compositions for which DTA measurements were performed. “C” and “H” mark compositional ranges of primary crystallization in the cubic or hexagonal phase, respectively.

Our findings motivated experiments on the growth of mixed sesquioxides by the Czochralski method. In a first attempt, a crystal with a melt-composition according to $(Er_{0.07}Y_{0.43}Sc_{0.5})_2O_3$ was grown by a Czochralski growth setup typically applied to high melting perovskite-structure scandate crystals [2]. Besides further reducing the melting point, the erbium-content was expected to make this material suitable as a gain material for laser operation in the 3 µm spectral range [3]. The outcome of this first growth run is shown in Fig. 2. The as-grown boule has a diameter of ~15 mm and a length of 40 mm. The crystal is clear and shows an intense pink color which is caused by the Er^{3+}-doping. A foot formation seen in the bottom part of the crystal is a known issue in the Czochralski growth of high-melting crystals and can be avoided in future by the use of proper seed crystals and improved thermal gradients. This result represents the first demonstration of the growth of high quality, large volume rare-earth sesquioxide crystals by the Czochralski method.

Application Science

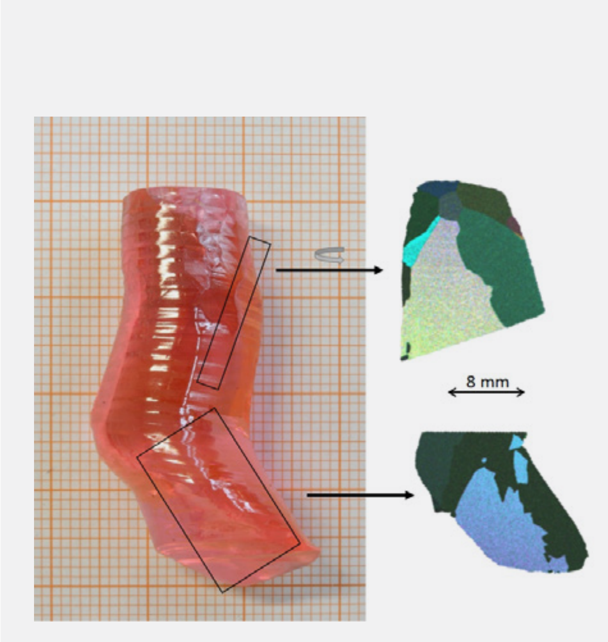

Fig. 2
Czochralski-grown $(Er_{0.07}Y_{0.43}Sc_{0.5})_2O_3$. The right side shows energy dispersive Laue mapping images taken on longitudinal cuts of the crystal from the sections indicated with black rectangles. Same colors indicate single crystalline regions.

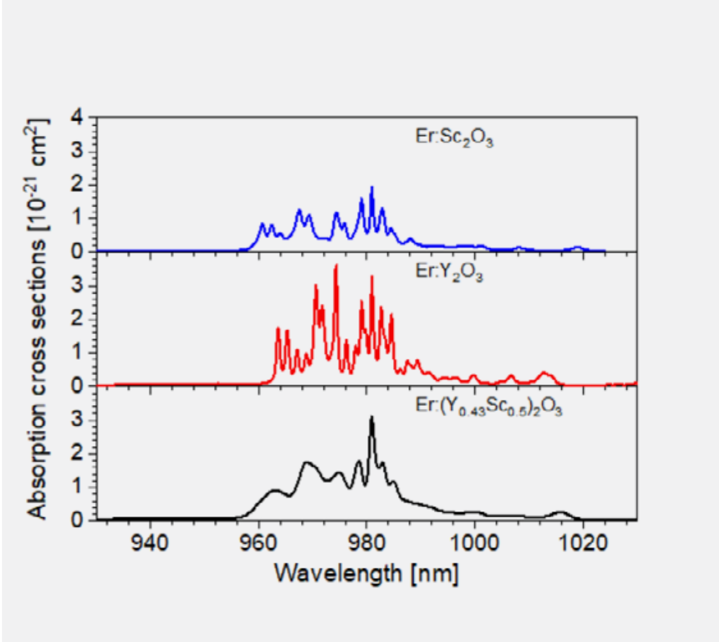

Fig. 3
Absorption spectra of $(Er_{0.07}Y_{0.43}Sc_{0.5})_2O_3$ compared to $Er:Sc_2O_3$ and $Er:Y_2O_3$.

Even though this first crystal was grown without a crystalline seed, the energy dispersive Laue mapping images shown in the right part of Fig. 2 indicate cm-scale single crystalline regions and a compositional analysis revealed a homogeneous composition of the crystal identical to the melt over its whole length. The cubic structure of this mixed crystal was confirmed by X-ray powder diffraction measurements. The disordered structure causes phonon scattering and thus a reduced thermal conductivity, but the room temperature value of 4.1 $Wm^{-1}K^{-1}$ is still higher than for other laser materials with comparable emission bandwidth. The absorption cross sections of the trivalent erbium ions in this crystal in the 1 μm range relevant for pump absorption in laser applications are shown in Fig. 3. Its disordered structure causes broadened spectra compared to pure Er^{3+}-doped sesquioxides and lasing at 2.85 μm has been achieved in initial experiments.

These results indicate that the growth of a variety of compositions of mixed sesquioxide crystals is possible by the Czochralski method. In particular when doped with trivalent ytterbium or thulium, these materials should exhibit outstanding properties as gain materials for high average power ultrashort-pulse lasers in the 1 μm and 2 μm spectral range, respectively. These findings have been filed as a patent [4] and enable for the first time a realistic perspective for a future commercial availability of high quality mixed cubic sesquioxide crystals.

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Appendix

Publications

Articles in international peer-reviewed journals

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Talks

Invited talks at national and international conferences

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F. Reichmann, J. Dabrowski, Z. Galazka, W. M. Klesse, M. Mulazzi, *Investigation of the Surface Electronic Structure of Bulk $ZnGa_2O_4$*, SPIE Photonics West, San Francisco, USA, 2020

T. Schröder, *Semiconducting ß-Ga_2O_3 films by MOVPE for future power electronics*, Workshop „Oxide Materials and Devices“, Xi‘an, China, 2020

J. Schwarzkopf, L. von Helden, D. Braun, M. Hanke, S. Liang, R. Wördenweber, M. Schmidbauer, *Strain engineering in (K,Na)NbO_3 epitaxial films for ferro-/piezoelectric applications*, Workshop ,,Oxide Materials and Devices", Xi'an, China, 2020

K. Stolze, C. Frank-Rotsch, *Semiconductor Single Crystals –Defect Reduction in Bulk Crystal Growth*, DGKK Seminar, Munich, Germany, 2020

M. Zupancic, T. Markurt, W. Aggoune, K. Char, Y. M. Kim, Y. Kim, C. Draxl, M. Albrecht, *Structural analysis of the polar – nonpolar $LaInO_3$/$BaSnO_3$ perovskite oxides interface*, Contributed (Oral) presentation at the Electronic Materials and Applications 2020 (EMA 2020) Orlando, Florida, USA, 2020

Invited seminars at national and international institutions

T. Schröder, *Innovative Crystalline Materials: Key Components for European Technology Sovereignty*, BMBF, Bonn, 2020

M. Bickermann, *Growth and Applications of Oxide and Fluoride Bulk Crystals at IKZ*, Seminar der Abteilung Methoden zur Charakterisierung von Transportphänomenen in Energiematerialien des HZB, Berlin, Germany, 2020

Talks

Oral contributions at national and international conferences

T. Straubinger, Growth of bulk AlN crystals – influence of the temperature field on growth rate, optical absorption and dislocation density, Annual German Growth Conference DGKK/DKT, Munich, Germany, 2020

A. Enders-Seidlitz, J. Pal, K. Dadzis, *Validation of a thermal crystal growth model including the effect of gas convection,* Leibniz MMS Online Symposium on Computational and Geophysical Fluid Mechanics, Online, 2020

R. Radhakrishnan Sumathi, R. Menzel, I. Buchovska, F. M. Kießling, R. Radhakrishnan Sumathi, T. Schröder, *IKZ's possibilities for contribution & co-operation to Einstein Telescope and 3GWD project*, Einstein-Telescope community workshop, Hannover, Germany, 2020

R. Radhakrishnan Sumathi, A. Gybin, K-P. Gradwohl, J. Janicskó-Csáthy, N. Dropka, U. Juda, J. Fischer, *Towards 80 mm dia, ultra-high purity germanium single crystals by Czochralski growth*, Annual German Crystal Growth Conference DGKK/DKT 2020), Munich, Germany, 2020

K-P. Gradwohl, A. Gybin, J. Janicsko-Csathy, M. Roder, A. N. Danilewsky and R. R. Sumathi, *Formation of vacancy related defects in high-purity germanium*, Annual German Crystal Growth Conference DGKK/DKT, Munich, Germany, 2020

K.-P. Gradwohl, O. Gybin, R. Radhakrisnan Sumathi, *Growth and defect investigation of high-purity germanium crystals for radiation detector applications*, 9th Annual Meeting of the Junge DGKK, Munich, Germany, 2020

K. Dadzis, R. Menzel, N. V. Abrosimov, *Numerical simulation of melt flow and species transport in silicon crystal growth*, the 14th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries, Trondheim, Norway (online), 2020

K. Dadzis, O. Pätzold, G. Gerbeth, *Model experiments for crystal growth*, Annual German Crystal Growth Conference DGKK/DKT, Munich, Germany, 2020.

K. Dadzis, *Crystal growth as a challenge for multi-physics coupling,* preCICE Workshop, Munich, Germany, 2020

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) KRISTMAG®

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) KRISTMAG®

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 KRISTMAG®

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 KRISTMAG®

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)

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

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 (Substrate for a semiconductor device, semiconductor device and method of manufacturing a substrate for a semiconductor device)
DE102020131850

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Patents

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 semi-conductor single crystals)
EP2504470B1 (NO, ES, NL, FR, DK, GB, BE, IT), DE102010052522B4, JP 5484589B2, US 9422636

Oxides

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

Z. Galazka, R. Uecker, D. Klimm, M. Bickermann
Method for growing beta phase of gallium oxide (ß-Ga_2O_3) single crystals from the melt contained within a metal crucible
EP3242965B1 (AT, BE, CH, DE, CZ, ES, FR, GB, IT, NL, PL), KR101979130B1, US20170362738A1

Z. Galazka, R. Uecker, R. Fornari
Method and apparatus for growing indium oxide (In_2O_3) single crystals and indium oxide (In_2O_3) single crystal
EP2841630B1 (DE, BE, FR, GB, IT), JP 6134379B2, US10208399

Aluminium nitride

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

A. Dittmar, C. Hartmann, J. Wollweber, U. Degenhardt, F. Stegner
Keimhalter einer Einkristallzüchtungsvorrichtung, Einkristallzüchtungsvorrichtung und Komposit-werkstoff
(Seed holder of a single crystal growth device, single crystal growth device and composite material)
DE102014017021A1

Oxides 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

Characterization

P. Gaal
Bereitstellen eines transienten Gitters
(Providing a transient grid)
DE102019132393, PCT/EP2020/082942

Semiconducting Layers/Nanostructures

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

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

Teaching and Education

Matthias Bickermann
Kristallzüchtung II: Methoden und Anwendungen
Technische Universität Berlin,
Institute of Chemistry

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

Christian Kränkel
Applied Photonics
Humboldt-Universität zu Berlin,
Department of Physics

Martin Schmidbauer
X-Ray Scattering:
Basics and Applications in Materials Science
Humboldt-Universität zu Berlin,
Department of Physics

Thomas Schröder,
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
Humboldt-Universität zu Berlin,
Department of Physics

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

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.; deputy executive committee spokesman

Conference Committees

C. Frank-Rotsch
- International Conference on Crystal Growth and Epitaxy ICCGE-20; member of the international advisory board
- 7th European Conference on Crystal Growth (ECCG7); member of the program committee

W. Miller
- International Conference on Crystal Growth and Epitaxy-ICCGE-20, member of the international advisory board
- 7th European Conference on Crystal Growth (ECCG7); member of the international scientific committee
- Deutsche Kristallzüchtertagung DKT 2021; member of the organization team

T. Schröder
- Workshop on Dielectrics in Microelectronics (WoDiM); member of the scientific advisory council
- Joint International SiGe Technology and Device Meeting (ISTDM) & International Conference on Silicon Epitaxy and Heterostructures (ICSI); member of the scientific advisory council

J. Schwarzkopf
- Electroceramics XVII; member of the scientific committee

R. Radhakrishnan Sumathi
- International Worskhop on Crystal Growth and Technology (IWCGT), Berlin; co-chair
- International Conference on Recent Trends in Applied Science and Technology (virtual) (ICRTAST); member of the scientific advisory committee

Other

T. Schröder
- Humboldt Universität zu Berlin/ Director Paul Drude Institut; member of the appointment committee
- Humboldt Universtität zu Berlin: Strategic committee of the Department of Physics; member
- TU Braunschweig, Professorship CMOS Design; member of the appointment committee
- BTU Cottbus-Senftenberg: Professorship Wireless Systems; member of the appointment committee
- Workgroup Gemeinsame Nutzung von Forschungsinfrastruktur (Shared Usage of Research Infrastructure) of the Berlin Senate Chancellery; member
- Leibniz Association project group on gender equality and management college on „Equality and Reconciliation“; member

R. Sumathi
- Vaibhav Summit 2020; expert panelist

Editorial committees

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

C. Kränkel
- Optics Express, associate editor

W. Miller
- Crystals, member of editorial board

Colloquia

Colloquia

PD Dr. Sebastian Fähler
“Epitaxial films as model systems to understand functional materials”
Leibniz-Institute for Solid State and Materials Research (IFW)
Dresden, Germany
January 20, 2020

Dr. Burkhard Beckhoff
“Characterization of advanced materials at the nanoscale by X-ray spectrometry using calibrated instrumentation”
“Characterization of advanced materials at the nanoscale by X-ray spectrometry using calibrated instrumentation”
Physikalisch-Technische Bundesanstalt, X-ray Spectrometry
Berlin, Germany
February 17, 2020

Prof. Dr. Hans-Joachim Freund
“Model Systems for Heterogeneous Catalysts at the Atomic Scale”
Fritz Haber Institut der Max Planck Gesellschaft
Berlin, Germany
February 21, 2020

Dr. Ruben Hühne
“Application of epitaxial oxide thin films for electrocaloric studies and strain engineering”
Leibniz-Institute for Solid State and Materials Research (IFW)
Institute for Metallic Materials
Dresden, Germany
February 24, 2020

Dr. Mathias Sander
“Ultrafast strain engineering of $SrTiO_3$“
Paul-Scherrer Institut
Villingen, Schwitzerland
September 21, 2020

Dr. Sánchez Florencio
Instituto de Ciencia de Materiales de Barcelona (ICMAB-CSIC)
Barcelona, Spain
September 28, 2020

Dr. Luca Ghiringelli
"Beyond Just Fitting Numbers: Interpretable Artificial Intelligence for the Small Data of Materials Science"
Fritz Haber Institut der Max Planck Gesellschaft
Berlin, Germany
October 12, 2020

Guest Scientists

Lee Ming-Hsun
10.02.2020 – 11.03.2020
University of Michigan, USA

Prof. Dr. Maki Hamada
09.10.2020 - 30.10.2021
Uni Kanazawa City, Japan

Dr. Humberto Foronda
10.05. – 30.12.2020
“Forschungsstipendiat
Alexander von Humboldt-Stiftung”

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