Annual Report

Leibniz-Institut für Kristallzüchtung

im Forschungsverbund Berlin e.V.

2019

ikz

Annual Report

Leibniz-Institut für Kristallzüchtung

im Forschungsverbund Berlin e.V.

2019

Preface

Sehr geehrte Leserinnen und Leser,

das Jahr 2019 brachte die offizielle Bestätigung der erfolgreichen Leibniz-Evaluation des IKZ, die wir in den vergangenen Jahren durch intensive Arbeit auf vielen Ebenen vorbereitet haben:
Der Senat der Leibniz-Gemeinschaft hat im Sommer 2019 die positive Förderempfehlung veröffentlicht, so dass die Zukunft unseres Instituts für die kommenden sieben Jahre innerhalb der Leibniz-Gemeinschaft gesichert ist. Mehr noch: Unsere neue, erweiterte IKZ Innovationsstrategie im Bereich Forschung & Entwicklung (F & E) zu kristallinen Materialien fand volle Unterstützung. In den kommenden Jahren wird es daher in unserer Verantwortung liegen, mit dieser Strategie die weltweit führende Vorreiterposition des IKZ als internationales Kompetenzzentrum für kristalline Materialien zu stärken.

Erste wichtige Maßnahmen wurden von uns bereits 2019 ergriffen, um diese Strategie in die Praxis umzusetzen! Um interdisziplinäre Forschungsaktivitäten zu fördern, haben wir das Institut im April 2019 durch vier neue wissenschaftliche Abteilungen in einer 2 x 2-Matrixstruktur neu strukturiert. Jede Abteilung besteht aus zwei zusammenhängenden Sektionseinheiten mit weiteren wissenschaftlichen Untergruppen.

Die Umstrukturierung betraf jedoch nicht nur die wissenschaftlichen Abteilungen, sondern auch die administrativen und technischen Dienste. Im administrativen Bereich haben wir insbesondere unser Team für Öffentlichkeitsarbeit zur Förderung der Kommunikation gestärkt. Für wichtige Aufgaben im Bereich Service & Transfer wurde die neue strategische Einheit Wissenschaftsmanagement eingerichtet. Im Hinblick auf die technischen Dienste haben wir unsere Techniker in einem Pool zusammengefasst, um flexibel auf die Bedürfnisse des Instituts einzugehen und einen Wissenstransfer zwischen den verschiedenen Einheiten zu intensivieren.

Das Jahr 2019 verzeichnete auch einen der größten wissenschaftlichen Erfolge in der Geschichte des Instituts: Am 20. Mai 2019, dem Welttag der Metrologie, wurde als letzter Schritt die weltweite Neudefinition der Masseneinheit Kilogramm (kg) eingeführt, um endlich alle sieben SI-Einheiten der Physik auf fundamentale Naturkonstanten zu beziehen. Die isotopenreinen & defektfreien ^{28}*Si-Kristalle des IKZ, die über viele Jahre unter der Projektleitung der Physikalischen Technischen Bundesanstalt (PTB) entwickelt wurden, bilden die Grundlage eines Ansatzes, der die etwa 130 Jahre alte, aber zu ungenaue kg-Definition auf der Basis eines Platinum-Iridium (Pt-Ir) Metallkörpers aus dem internationalen Büro für Maß und Gewicht (BIPM) in Sèvres ersetzt. Mit anderen Worten: Das IKZ ist der einzige Ort auf diesem Planeten, an dem diese Präzision bei der* ^{28}*Si-Kristallzüchtung erreicht wird. Die Kristalle aus unserem Institut beeinflussen somit das tägliche Leben eines jeden Menschen „maßgeblich“ über eine präzise Grundlage für die kg-Metrologie.*

Letztendlich ist die Qualifikation junger Menschen eine wichtige Aufgabe unseres Instituts, und ich möchte allen unseren leitenden Wissenschaftlern danken, die sich aktiv an den Aufgaben der Doktorandenausbildung beteiligen. Fünf junge Kollegen konnten im Jahr 2019 ihre Doktorarbeit mit besten Ergebnissen erfolgreich verteidigen und fanden Arbeitsplätze in unterschiedlichen Bereichen wie Industrie, Forschung, Bildung und Kommunikation. Fünf junge Nachwuchsforschergruppen haben auch 2019 ihre Arbeit zu strategischen Themen in verschiedenen Abteilungen aufgenommen, und ein erster beeindruckender Erfolg ist die Bewilligung des ersten ERC Grants des IKZ sowie ein großes ForMikro-Projekt des BMBF.
Bitte lesen Sie für weitere Details meinen ausführlicheren Bericht über das Jahr 2019 auf den folgenden Seiten.

Wir wünschen Ihnen eine informative & unterhaltsame Lektüre des IKZ-Jahresberichts 2019!

Mit freundlichen Grüßen

Thomas Schröder

Preface

Dear Readers,

the year 2019 brought the official confirmation of IKZ´s successful Leibniz evaluation which we prepared over the past years by intensive work on many levels: The Senate of the Leibniz Association published in Summer 2019 the positive funding recommendation so that our institute´s future is secured for the coming seven years within Leibniz. Even more, our new extended IKZ research & development (R & D) innovation strategy in the area of crystalline materials became fully supported. In the coming years, it will thus be our responsibility to work along these strategy guidelines to strengthen IKZ´s worldwide leading flagship position as international center of competence for crystalline materials.

First important action was already taken by us in 2019 to put this strategy in practice ! To promote interdisciplinary research activities, we restructured the institute in April 2019 by four new scientific departments in a 2 x 2 matrix structure. Each department is composed of two related section units with further scientific sub-groups. The restructuring however did not only affect the science departments but also administrative and technical services. In the administrative area, we consolidated in particular our public relation team to promote communication and established our new strategic science management unit for important tasks in service & transfer. With respect to the technical services, we grouped our technicians into a pool to serve the needs of the institute in a flexible way and create knowledge transfer across different units.

The year 2019 also marked one of the biggest scientific successes in the institute´s history: On 20th May 2019, the world day of metrology, the new worldwide definition of the kilogram (kg) mass unit was put in place as last step to finally relate all seven SI units in physics to fundamental natural constants. IKZ´s isotope pure & defect free ^{28}Si crystals, developed over many years of R & D under the project guidance of the German "Physikalische Technische Bundesanstalt (PTB)", form the very basis of one approach to replace the about 130 year old, but too inaccurate kg definition based on a Pt-Ir metal body which is stored at the International Bureau of Weights and Measures in Sèvres. In other words: IKZ is the only place on this planet to achieve this precision in ^{28}Si crystal growth and crystals from our institute thus fundamentally influence everybody´s daily life.

Finally, qualification of young people is an important task of our institute and I wish to thank all our senior scientists actively engaged in Phd graduation tasks. Five young colleagues could successfully defend their PhD work with best results in 2019 and found jobs in fields as different as industry, research, education & communication. Five young junior research groups started furthermore their work in 2019 on strategic topics in different departments and first impressive success is given by the approval of IKZ´s first ERC grant plus a big BMBF ForMikro project. Please consult for further details my more detailed report on the year 2019 on the following pages.

We wish you an informative & entertaining lecture of IKZ´s Annual Report 2019 !

With best regards

Thomas Schroeder

Content

The Institute

Photo: Lothar M. Peter © IKZ

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 sowie 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 co-operation 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 Schlüsseltechnologien

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

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

Materialien

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

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

- Silizium-Kristalle für Mikro- und Leistungselektronik und Photovoltaik

- Isotopenreine Halbleiter (Silizium und Germanium) für die Quantentechnologie

- Galliumarsenid für die drahtlose Kommunikation und in Hochfrequenztechnik

- 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 photonics

- Prototype supply of innovative crystals up to small-scale batches – with tailored properties and specifications – for reliable technology research, including preparations for market introduction

- Development of wafering processes for new materials, fine processing of special optical crystals.

Materials presently in development:

- 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 micro- and 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 verpflichtet. In den folgenden drei Jahren haben wir die in diesem Prozess definierten Maßnahmen umgesetzt. Die Zertifizierung wurde 2018 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

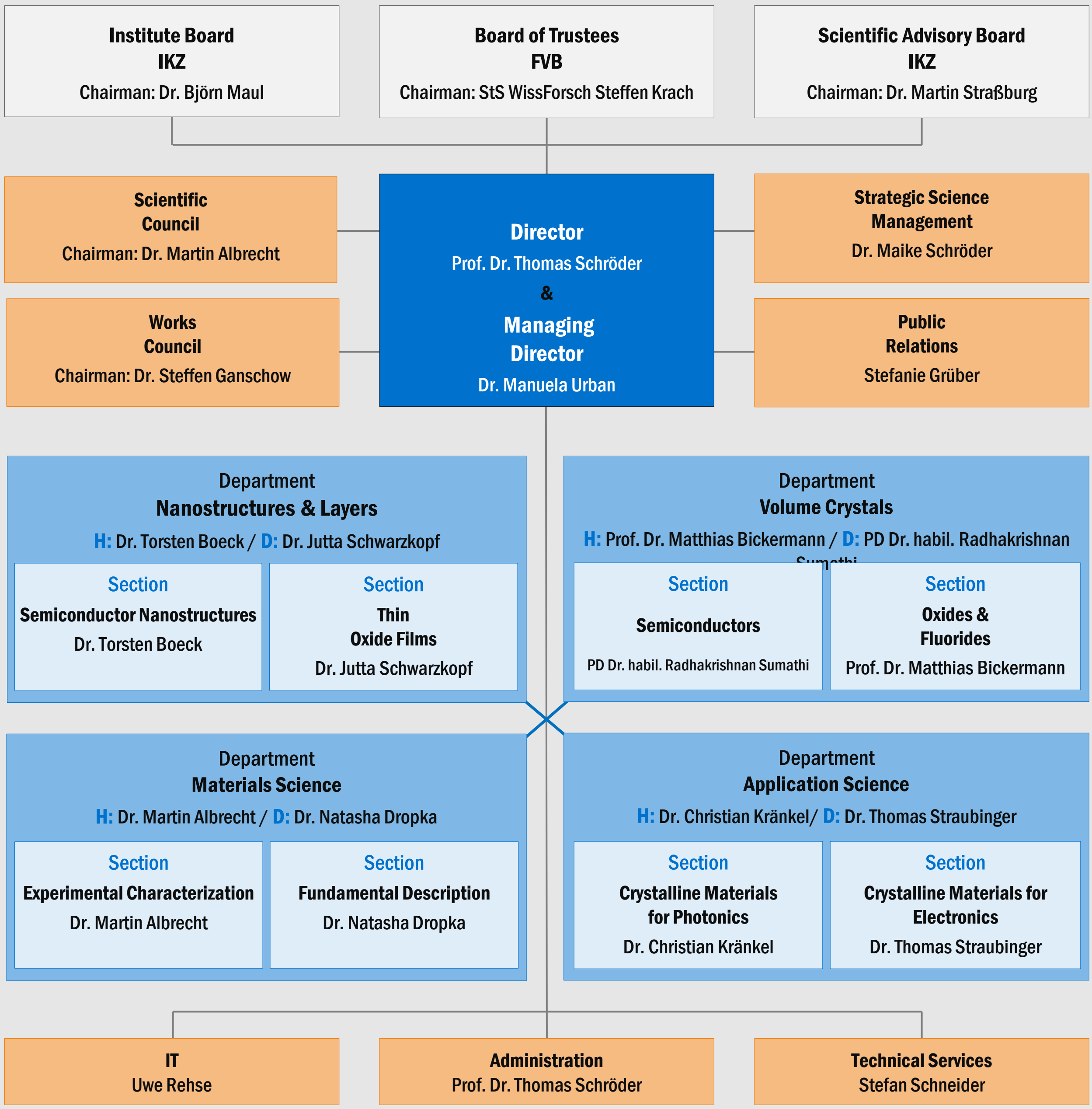
The institute intends to create a co-operative and open working environment for all employees. It places special emphasis on the reconcilability of job and family, offering flexible working time models as well as full or part-time employments. In 2015, the institute has been awarded the *audit berufundfamilie* 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.

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 www.beruf-und-familie.de

Zertifikat seit 2015
audit berufundfamilie

The Institute

Organigramm 2019
Organisation Chart 2019



Wissenschaftlicher Beirat 2019
Scientific Advisory Board 2019

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

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

Dr. Hubert Aulich
SC Sustainable Concepts GmbH,
Erfurt, Germany

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

Prof. Dr. Michael Kneissl
Institute of Solid State Physics,
Technische Universität Berlin,
Berlin, Germany

Prof. Dr. Darrell Schlom
Cornell University,
Department of Materials Science and Engineering,
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

2019 – das Jahr der Neustrukturierung des IKZ für seine erweiterte F & E-Strategie

2019 – the year of IKZ's reorganization for its new extended R & D strategy

Sehr geehrte Leserinnen und Leser,

das Jahr 2019 war ausgelastet mit vielen Aktivitäten in Wissenschaft und Technik sowie in administrativen und technischen Bereichen. Es ist mir eine große Freude, mit vielen engagierten IKZ-Mitarbeiter*innen auf all diesen verschiedenen Ebenen zusammenzuarbeiten, um unser Institut voranzubringen. Bevor ich zu den Einzelheiten komme, möchte ich Ihnen allen für die hochqualifizierte Arbeit danken, die im Jahr 2019 geleistet wurde!

Der Kürze halber konzentriere ich mich im Folgenden in meinem Jahresrückblick auf die Managementprozesse im Jahr 2019, um die Arbeit der technischen und administrativen Mitarbeiter*innen zu würdigen; die Wissenschaft überlasse ich den Kapiteln der wissenschaftlichen Abteilungen, die in kurzen und prägnanten Artikelbeiträgen die Höhepunkte ihrer Forschungs- und Entwicklungsarbeit (F & E- Arbeit) ansprechend darstellen.

Erfolgreiche Leibniz-Evaluierung

Die wichtigste Botschaft traf zweifellos im Juli 2019 vom Senat der Leibniz-Gemeinschaft ein. Es war die offizielle Bestätigung der erfolgreichen Leibniz-Evaluierung des IKZ. Damit haben wir erneut die Zukunft des IKZ innerhalb der Leibniz-Gemeinschaft für die kommenden sieben Jahre gesichert! Die Kommission war tief beeindruckt von der wissenschaftlichen, technischen und administrativen Arbeit, die in der Vergangenheit geleistet wurde. Die Kommission machte deutlich, dass dieser Erfolg in der langen Übergangszeit des fehlenden Direktors erreichbar wurde, da sehr engagierte Mitarbeiter oft deutlich über ihre ursprünglichen Aufgaben hinaus Verantwortung übernahmen. Ich danke Ihnen allen für dieses Engagement für unser Institut in der vergangenen Evaluationsperiode!

Erweiterte IKZ-Innovationsstrategie

Mit Blick auf die Zukunft wurde unsere neue, erweiterte IKZ-Innovationsstrategie im Bereich F & E auf dem Gebiet der kristallinen Materialien von der Leibniz-Gemeinschaft voll unterstützt. Diese Strategierichtlinien - zur Stärkung der weltweit führenden Vorreiterposition des IKZ als internationales Kompetenzzentrum für kristalline Werkstoffe - werden somit in den kommenden Jahren von uns in die Praxis umgesetzt. Selbstverständlich ist eine Strategie ein dynamischer und kein statischer Prozess, so dass wir uns ständig flexibel anpassen müssen, um die anstehenden F & E- Möglichkeiten voll auszuschöpfen.

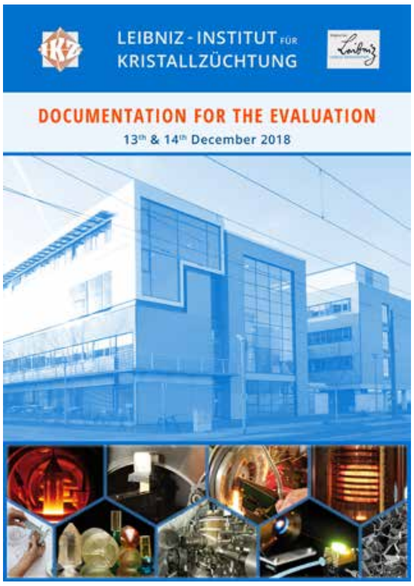
Dear Readers,

the year 2019 was filled with many activities in science & technology as well as in administrative & technical services. It is my great pleasure to work with many committed IKZ staff members on all these various levels to push our institute ahead. Before moving to details, let me thank you all for the highly qualified work done in 2019!

In the following, for the sake of shortness, I focus my review of the year on management processes in 2019 to honor the work done by technical and administrative staff; I leave the science to the scientific department chapters which nicely present the highlights of their R & D work in short and concise article contributions.

Successful Leibniz evaluation

Without doubt, the most important message arrived in July 2019 from the Senate of the Leibniz Association. and was the official confirmation of IKZ´s successful Leibniz evaluation. Again, we secured IKZ´s future within the Leibniz Association for the coming seven years! The commission was deeply impressed by the scientific, technical and administrative work done in the past. The commission clearly stated that this success only became possible in the long interim time of the missing director due to the fact that a very dedicated staff often took over responsibilities clearly beyond their original job duties. Thank you all for that commitment for our institute over the past evaluation period!



Evaluierungsunterlagen

Documentation for the evaluation

The Institute

Gemäß des zweistufigen Konzepts, welches im Leibniz-Evaluierungsabschlussbericht definiert wurde, um diese Strategie mit Aktivitäten zu füllen, haben wir den ersten Schritt bereits 2019 getan. Um eine nützliche Managementstruktur für interdisziplinäre F & E zu schaffen, wurde das Institut im April 2019 neu organisiert. Vier wissenschaftliche Abteilungen, die in einer 2 x 2- Matrixstruktur angeordnet sind, bilden nun das eigentliche wissenschaftliche Zentrum unseres Instituts. Jede Abteilung ist durch zwei verwandte, aber wissenschaftlich unabhängige Sektionen (mit jeweils weiteren wissenschaftlichen Untergruppen) gekennzeichnet. Ein Charakteristikum des IKZ ist somit die Doppelspitze jeder wissenschaftlichen Abteilung, die es uns ermöglichte, durch eine bessere Verteilung der administrativen Managementaufgaben, neben der Wissenschaft, exzellente Wissenschaftlerinnen für diese zweite Führungsebene zu gewinnen. Interessanterweise weist das IKZ auf der ersten und zweiten Führungsebene somit ein Geschlechterverhältnis von nahezu 50:50 auf, was ein sehr positives Ergebnis für jedes F & E-Institut im Bereich der Naturwissenschaften mit starker Betätigung im Bereich der Technologieentwicklung ist.

Neuorganisation des IKZ

Diese Neuorganisation des IKZ im April 2019 betraf nicht nur die wissenschaftlichen Abteilungen, sondern umfasste auch administrative und technische Dienstleistungen zur Modernisierung unseres Hauses. In dieser Hinsicht wurde das Team für Öffentlichkeitsarbeit zur Förderung der Kommunikation innerhalb und außerhalb des Instituts umfassend eingerichtet. Zum Beispiel wurde der monatliche IKZ-Newsletter zu unserem zentralen Instrument, um alle über Aktivitäten und Veranstaltungen im IKZ zu informieren. Sehr wichtig ist, dass unsere Einheit Strategische Wissenschaftsmanagement personell verstärkt wurde, um wichtige Aufgaben im Bereich Service & Transfer zu bewältigen. Hier ermöglicht uns die zentrale Proben-Versandstelle, mit den aktuellen Exportbestimmungen kompatibel zu bleiben und unsere Geschäftstätigkeit in Bezug auf Steuerfragen aufzuzeichnen. Eine weitere wichtige Aufgabe bestand darin, unsere Techniker in einem technischen Servicepool zusammenzufassen, um flexibel auf die Bedürfnisse des Instituts eingehen zu können und einen Wissenstransfer zwischen verschiedenen internen Einheiten zu schaffen. Letzteres ermöglicht es den Mitgliedern des technischen Dienstes, ihre Fähigkeiten in einem breiteren Spektrum von Möglichkeiten zu entwickeln, und die Leitung des IKZ kann die Infrastruktur des Hauses mit einem hochqualifizierten Stammpersonal auf zuverlässigere Weise unterstützen („second in the row regulations"). Unsere Verwaltung war 2019 sehr aktiv bei Digitalisierungsprojekten, um die Prozesse im IKZ und im FVB effizienter zu gestalten. Die „Smart Time Software", als elektronische Plattform für das Zeitmanagement, wurde erfolgreich eingeführt und beseitigte die alten Papierformulare.

New extended IKZ research & development (R&D) innovation strategy

Looking into the future, our new extended IKZ research & development (R & D) innovation strategy in the area of crystalline materials became fully supported by the Leibniz Association. These strategy guidelines – to strengthen IKZ´s worldwide leading flagship position as international center of competence for crystalline materials - will thus be put in practice by us in the coming years. Certainly, strategy is a dynamic and never a static process so that we will continuously need to readjust in order to make full use of upcoming R &D opportunities.

According to the two step roadmap defined in the Leibniz evaluation documents to fill this strategy with activity, the first step was already taken by us in 2019. To set up a useful management structure for interdisciplinary R & D, the institute was reorganized in April 2019. Four scientific departments organized in a 2 x 2 matrix structure form now the very scientific center of our institute. Each department is characterized by two related but scientifically independent sections (with further scientific sub-groups each). An IKZ characteristic is thus the dual leadership of each scientific department which allowed us – by a better distribution of administrative management load besides the science to do – to win excellent female scientists for this second management level. Interestingly, IKZ has on the first and second management level thus a gender balance of close to 50:50 which is a very positive result for any R & D institute in the field of natural sciences with a strong impact on technology development.

Reorganization of the IKZ

This reorganization of IKZ in April 2019 did not only affect the scientific departments but included also administrative and technical services to modernize our governance. In this respect, the public relation team to promote communication inside and outside the institute became fully established. For example, the monthly IKZ Newsletter became our central tool to inform everybody about activities and events at IKZ. Very important, our strategic science management unit became strengthened to cope with important tasks in service & transfer. Here, the central sample dispatch office allows us to stay compatible with current export rules and monitor our business activity with respect to tax issues. Another important job to be done was to group our technicians into a technical service pool to serve the needs of the institute in a flexible way and create knowledge transfer across different in-house units. The latter allows the members of the technical services to develop their skills in a broader range of opportunities and IKZ management can provide infrastructure support with a highly skilled permanent staff in a more reliable way ("second in the row regulations").

The Institute

Eine größere Herausforderung ist das „*Administrative Intelligence (AI) System*“: Es wurde erfolgreich eingeführt, um unsere Einkaufsaktivitäten und öffentlichen Ausschreibungsprozesse rechtskonform zu den heutigen EU-Gesetzen anzupassen. Trotz der ausgezeichneten Unterstützung durch die Kolleg*innen der Gemeinsamen Verwaltung des FVB ringen wir jedoch immer noch mit den oft zu zeitaufwendigen Prozessanforderungen, so dass eine Verbesserung noch erforderlich ist. Die IT-Abteilung unterstützte all diese Digitalisierungsprozesse auf professionelle Art und Weise. Ein wichtiger Schritt im IT-Bereich war darüber hinaus die Einführung von etwa 60 Laptops für unsere Mitarbeiter*innen, um die Datenverarbeitung im IKZ professioneller zu gestalten. Datensicherheit, basierend auf den neuen Datenverordnungsgesetzen, ist ein wichtiges Thema für jedes F & E- Institut mit Ambitionen auf eine moderne Technologieentwicklung. Diese Hardware-Basis ist ein wichtiger Meilenstein, um flexible Arbeitsbedingungen zu ermöglichen und trotzdem die IKZ Daten unter der Kontrolle des Arbeitgebers zu verwalten. Zusätzlich wurde in enger Zusammenarbeit mit dem IKZ-Betriebsrat und unserem Datenschutzbeauftragten eine moderne IT-Regelung geschaffen, um diesen wichtigen Maßnahmenpunkt abzuschließen. Künftig investieren wir im IKZ in unsere WLAN-Zugangsstellen, um diese moderne IT-Plattform in vollem Umfang nutzen zu können. *Last but not least* haben wir in enger Zusammenarbeit mit dem Betriebsrat des IKZ eine moderne Arbeitgeber-/Betriebsratsvereinbarung abgeschlossen, um die Arbeitsbedingungen im IKZ für alle Mitarbeiter*innen flexibel und zeitgemäß zu regeln.

Sondertatbestand „Kristalltechnologie“

Der zweite Schritt, der in der Leibniz-Empfehlung des IKZ zur Umsetzung der neuen Strategie vorgesehen ist, betrifft die Gewährung unseres kleinen spezifischen Sondertatbestands „Kristalltechnologie“. Dieses interdisziplinäre Forschungsprogramm wird die Strategie des IKZ in Richtung auf die zuverlässige Bewertung und das Benchmarking ausgewählter Kristallsysteme für die Technologieentwicklung - in enger Zusammenarbeit mit Instituten für technologische Forschung und Entwicklung (z.B. Mitglieder der „Forschungsfabrik Mikroelektronik Deutschland (FMD)“) und Industrieunternehmen – erweitern. Das Verwaltungsverfahren zur Genehmigung dieses Sondertatbestandes in der Leibniz-Gemeinschaft ist langwierig und komplex; es erfordert etwa sieben verschiedene Zustimmungen hochrangiger Gremien! Nach voller Unterstützung durch den Wissenschaftlichen Beirat & Institutsrat des IKZ, die Leibniz-Evaluationskommission und das Kuratorium des FVB hat das Land Berlin der Einreichung unseres Antrags bei der Gemeinsamen Wissenschaftskonferenz (GWK) hohe Priorität eingeräumt.

Our administration was very active in 2019 on digitalization projects to make IKZ and FVB processes more efficient. The “Smart Time Software” as electronic platform for time management became successfully introduced and removed the old paper forms. More challenging is the ´Administrative Intelligence (AI)` system: It was successfully introduced to make our purchase activities and public tender processes legally compliant to today´s EU laws. However, despite excellent support by colleagues from the FVB Joint Administration, we are still struggling on its often too time consuming process requirements so that improvement is mandatory. The IT unit supported all these digitalization processes in a professional way. An important step in IT was furthermore the introduction of about 60 labtops to our staff to make data handling at IKZ more professional. Data security, based on the new data regulation laws, is an important issue for any R & D institute with ambition on modern technology development. This hardware basis is an important milestone to allow for flexible work conditions but keep IKZ data under the employer´s control; a modern IT regulation was set up in addition in close collaboration with IKZ work council and our data security officer to complete this important action point. In future, we invest on our WLAN access points at IKZ to make full use of this modern IT platform. Last but not least, in close collaboration with IKZ´s work council, we set up a modern employer / work council agreement to regulate work conditions at IKZ in a flexible and modern way for all our staff.

Item of expenditure “Crystal Technology”

The second step, foreseen by IKZ´s Leibniz recommendation to implement the new strategy, concerns the granting of our extraordinary item of expenditure called “Crystal Technology”. This interdisciplinary research program will extend IKZ´s strategy towards the reliable evaluation and benchmarking of selected crystal systems for technology evaluation in close collaboration with technology R & D institutes (e.g. members of the ´Forschungsfabrik Mikroelektronik Deutschland (FMD)`) and industry companies. The administrative procedure for approval of these extraordinary items of expenditure in the Leibniz Association is lengthy and complex; it requires around seven different committee votes! After full support by IKZ´s scientific advisory council & institute board, the Leibniz evaluation commission and the FVB board of trustees, the State of Berlin gave high priority to the submission of our proposal to the German Joint Science Conference. Unfortunately, a procedural error occurred in the Leibniz-Senate Strategic Committee which resulted in the fact that IKZ´s proposal could not enter into the competitive evaluation by the German Joint Science Conference.

The Institute

Leider ist im Strategischen Ausschuss des Leibniz-Senats ein Verfahrensfehler aufgetreten, der dazu führte, dass der Antrag des IKZ nicht in die wettbewerbliche Bewertung durch die GWK eingehen konnte. Sicherlich stellt diese Situation eine Herausforderung für die professionelle und fristgerechte Umsetzung unserer neuen erweiterten institutseigenen F & E- Strategie dar; wir stehen heute in engem Kontakt mit dem Leibniz-Präsidenten sowie den Fördereinrichtungen von Land und Bund für eine schnelle Wiedervorlage unseres Forschungsprogramms „Kristalltechnologie" im Jahr 2020.

„Kampf ums Geld"

Der „Kampf ums Geld" ist eine intensive Aufgabe für jedes moderne F & E- Institut. Das IKZ gehört derzeit zu den besten im FVB e.V. und bezogen auf das Gesamtbudget haben wir 2019 einen Drittmittelanteil von ~30 % erreicht. Dies ist ein sehr konkurrenzfähiges Ergebnis und erfordert die Aufmerksamkeit des Direktors und vieler führender Wissenschaftler*innen, um in Zukunft auf diesem hohen Niveau voranzukommen. Wir haben Fördergespräche mit leitenden Wissenschaftlern und Förderbetreuungsgespräche mit Nachwuchswissenschaftlern - jeweils im zweimonatigen Wechsel – eingerichtet. Diese Treffen dienen einerseits einem koordinierten, transparenten Einreichungsprozess unserer Anträge und andererseits einer ausreichenden Finanzkontrolle für unsere Wirtschaftsplanung am IKZ. Neben akademischen Partnern ist das IKZ sehr aktiv in der Zusammenarbeit mit Industriepartnern. Persönlich nutze ich viele Dienstreisen, um Verbindungen zu Unternehmen herzustellen und zu fördern. Im Jahr 2019 ist das Ergebnis sehr positiv, und wir haben öffentlich geförderte bzw. bilaterale F & E- Verträge abgeschlossen mit Firmen wie FCM, Siltronic, Saint Gobain, EOT, Crystec, Bestec, G-Ray, Kistler AG, IBM, Aixtron, ABB usw. Ziel dieser F & E- Arbeiten für unsere Industriepartner ist stets, mit unserer Expertise oftmals im Bereich der Grundlagenfragen, die Entwicklung des zukünftigen Produktportfolios zu unterstützen.

Neudefinition der Maßeinheit Kilogramm

Wir freuen uns sehr, im Folgenden über einen der größten wissenschaftlichen Erfolge in der Geschichte unseres Instituts berichten zu können, der am 20. Mai 2019, dem Welttag der Metrologie, angekündigt wurde: Die weltweite Neudefinition der Maßeinheit Kilogramm (kg) wurde eingeführt; es war der letzte Schritt, endlich alle sieben SI-Einheiten der Physik auf fundamentale Naturkonstanten zu beziehen (anstelle der bisherigen Verwendung künstlicher Objekte).

Certainly, this situation challenges the professional and timely implementation of our new extended institute R & D strategy; today we are in close contact with the Leibniz president as well as state and federal funding bodies for a fast resubmission of our research program "Crystal Technology" in 2020.

"Fighting for money"

"Fighting for money" is an intensive job for any modern R & D institute. IKZ is currently among the best in the FVB e.V. and, with respect to the total budget, we achieved in 2019 a third party funding share of ~30 %. This is a very competitive result and requires attention by the director and many leading scientists to move ahead on this high level in future. We established funding meetings with senior scientists and funding mentoring meetings with junior researchers – each every two months in an alternating way – to achieve on the one hand a coordinated, transparent proposal submission process and on the other hand sufficient finance control for our planning at IKZ. Besides academic partners, IKZ is very active on collaborations with industry partners. Personally I dedicate a lot of business trips to establish and promote links to companies. In 2019, the result is very positive and, either by public or bilateral R & D contracts, we signed contracts with companies like FCM, Siltronic, Saint Gobain, EOT, Crystec, Bestec, G-Ray, Kistler AG, IBM, Aixtron, ABB etc. to support R & D work for our industrial partners on the development of their future product portfolio.

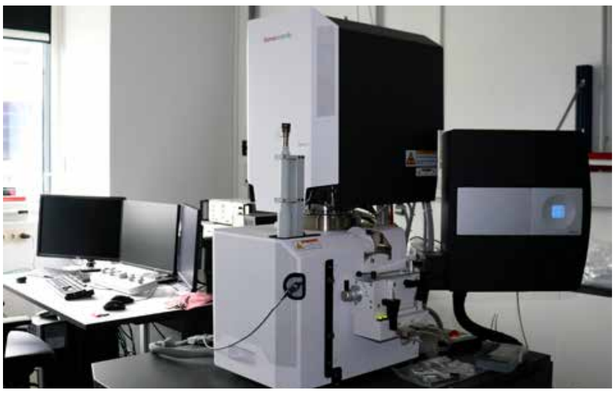
Si-Kugel mit Gruppenspiegelung
Si-sphere with group mirroring

The Institute

Die isotopenreinen & defektfreien ^{28}Si-Float-Zone (FZ)-Kristalle des IKZ, die in langjähriger Forschungs- und Entwicklungsarbeit unter der Projektleitung der „Physikalischen Technischen Bundesanstalt (PTB)" – zusammen mit wichtigen Partnern aus Russland - entwickelt wurden, bilden nun die Grundlage für einen von zwei Ansätzen zur genauen Definition der Maßeinheit kg. Diese ultrapräzisen ^{28}Si-Kristallkugeln ersetzen damit die etwa 130 Jahre alte, aber zu ungenaue kg-Definition auf der Basis eines im Internationalen Büro für Maß und Gewicht (BIPM) in Sèvres ausgestellten Platinum-Iridium (Pt-Ir)- Metallkörpers. Mit anderen Worten: Das IKZ ist das einzige Institut auf der Welt, das diese Präzision in der ^{28}Si-Kristallzüchtung erreicht, und die Kristalle unseres Instituts beeinflussen somit „maßgebend" das tägliche Leben eines jeden Menschen durch präzise Messtechnik.

Qualifizierung von Nachwuchs

Eine weitere wichtige Rolle des IKZ ist die Qualifizierung von naturwissenschaftlichem Nachwuchs für zukünftige Tätigkeiten in den verschiedensten Bereichen wie Wissenschaft, Technik, Industrie, Verwaltung, Kommunikation etc. Unser Dank gilt allen unseren leitenden Wissenschaftler*innen, die sich aktiv an diesen Bildungs- und Lehraufgaben beteiligen. Im Jahr 2019 verteidigten fünf Doktoranden erfolgreich ihre Doktorarbeit mit besten Ergebnissen und fanden Arbeitsplätze in so unterschiedlichen Bereichen wie Industrie, Forschung, Bildung & Kommunikation. Wir haben einen weiteren langfristigen Weg eingeschlagen, um die Karriere unseres wissenschaftlichen Nachwuchses zu fördern: Wir stellten strategische Themen in verschiedenen Abteilungen fest und richteten 2019 am IKZ fünf Nachwuchsforschergruppen ein. Diese Nachwuchsforscherinnen und -forscher erhalten eine stabile Vertragssituation von fünf (3+2) Jahren; es wird erwartet, dass sie durch Drittmittel eine Gruppe aufbauen und sich durch Wissenschaft auf hohem Niveau international einen Namen machen. Ein erster beeindruckender Erfolg ist die Bewilli-gung des ersten *„ERC Starting Grants"* des IKZ sowie eines *„BMBF-ForMikro-Projekts"* für zwei unserer Nachwuchsforscher.



Elektronenmikroskopie-Labor
Electron Microscopy Laboratory

New definition of the kilogram

In the following, we are very delighted to report on one of the biggest scientific successes in our institute´s history which was announced on 20th May 2019, the world day of metrology: The new worldwide definition of the kilogram (kg) mass unit was put in place; it was the last step to finally relate all seven SI units in physics to fundamental natural constants (instead of the former use of artificial objects).

IKZ´s isotope pure & defect free ^{28}Si Float zone (FZ) crystals, developed over many years of R & D under the project guidance of the German "Physikalische Technische Bundesanstalt (PTB)" – together with important partners from Russia-, form now the very basis of one out of two approaches to precisely define the kg mass unit. These ultra-precise ^{28}Si crystal spheres thus replace the about 130 year old, but too inaccurate kg definition based on a Pt-Ir metal body exposed in the International Bureau of Weights and Measures in Sèvres. In other words: IKZ is the only institute on earth to achieve this precision in ^{28}Si crystal growth and crystals from our institute thus fundamentally influence everybody´s daily life by precise metrology.

Qualification of young talents

Qualifying skilled young staff for future jobs in a wide range of opportunities like science, technology, industry, administration, communication etc. is another important role of IKZ. Thanks to all our senior scientists actively engaged in these education & teaching tasks. In 2019, five PhD students successfully defended their PhD work with best results and found jobs in fields as different as industry, research, education & communication. We embarked on the establishment of a further long-term way to promote our young researcher´s career: We identified strategic topics in various departments and established five junior research groups in 2019 at IKZ. These junior researchers receive a stable contract situation on a scale of five (3+2) years; they are expected to build up a group by third party funds and establish an international reputation by high level science. First impressive success is given by the approval of IKZ´s first ERC starting grant plus a BMBF ForMikro project to two of our junior researchers.

"Outreach" activity

To promote our R & D community beyond IKZ staff, we organized a Summer School in September 2019 on "Quantum Computing as a Material Challenge" (Lecturer: Prof. Lars Schreiber / FZ Jülich) and a Winter School "International Lecture on Crystal Growth" (Lecturer: Prof. Peter Rudolph / CTC Berlin).

The Institute

„Outreach"-Aktivitäten

Um unsere F & E- Gemeinschaft über die IKZ-Mitarbeiter hinaus zu fördern, organisierten wir im September 2019 eine *Summer School* zum Thema „Quantum Computing as a Material Challenge" (Dozent: Prof. Lars Schreiber / FZ Jülich) und eine *Winter School* „International Lecture on Crystal Growth" (Dozent: Prof. Peter Rudolph / CTC Berlin). Beide Veranstaltungen waren ausgebucht und das Publikum umfasste sowohl Kolleg*innen aus akademischen Forschungsinstituten als auch aus führenden Kristallzüchtungsfirmen. Das IKZ wird auch in Zukunft diese wichtige „*outreach*"-Aktivität weiterführen.

Unsere Technischen Dienste sind sehr aktiv bei der Modernisierung unserer Institutseinrichtungen. Die Hauptaktivität ist den Laborumbauten gewidmet, um eine moderne und sichere Infrastruktur zu schaffen. Viele Laboratorien wurden mehr als ein Jahrzehnt lang nicht modernisiert. So haben wir zum Beispiel ein leistungsfähiges „Reinst-Germanium (HP-Ge)-Labor" eingerichtet, das nicht nur CZ-Wachstumseinrichtungen, sondern auch GeO_2-Reduktionsöfen und Zonenreinigungsanlagen (mit Optionen für die Behandlung unter Wasserstoffatmosphäre) umfasst. Ein weiteres Beispiel ist das hochmoderne neue Elektronenmikroskopielabor, das jetzt voll funktionsfähig ist. Trotz der Schwierigkeiten, die heutzutage bei öffentlichen Ausschreibungen und bei der Suche nach Bauunternehmen auftreten, bin ich immer wieder beeindruckt, dass die Übergabe der Labors zurück an die Wissenschaft fast immer rechtzeitig und im Rahmen des vorgesehenen Finanzbudgets erfolgt. Großartige Arbeit!

Institutsexkursion Beelitzer Heilstätten

Die Technischen Dienste organisierten auch unsere Institutsexkursion des IKZ am 09. September 2019 zu *den* „Beelitzer Heilstätten" in Brandenburg. An diesem Tag zog eines der Hauptregenfelder des Jahres 2019 über Brandenburg hinweg, was sogar zu Verkehrsbehinderungen im deutschen Schienennetz führte. Trotz allem hatten wir, dank perfekter Organisation, einen sehr unterhaltsamen & interessanten Rundgang zur Geschichte der beeindruckenden Bebauung und mit einem perfekten Barbecue unter den Dächern einiger Zelte.

Genießen Sie eine inspirierende Lektüre des IKZ-Jahresberichts 2019. Falls Sie Fragen haben, zögern Sie nicht, uns zu kontaktieren und wir werden Ihre Fragen gerne beantworten.

Mit freundlichen Grüßen
Thomas Schröder

Both events were fully booked and the audience included colleagues from academic research institutes as well as from leading crystal growth companies. IKZ will move ahead in future to maintain this important "outreach" activity.

Our Technical Services are very active to modernize our institute facilities. Major activity is devoted to laboratory refurbishments to set up modern and safe infrastructure. Many laboratories were not upgraded for more than a decade. For example, we set up a powerful "Hyper-pure Germanium (HP-Ge)" laboratory which includes not only CZ growth facilities but also GeO_2 reduction ovens and zone refining equipment with options for treatment in hydrogen atmosphere. Another example is given by the state-of-the-art new electron microscopy laboratory which is now fully functional. I am always impressed, despite the difficulties of public tenders and finding companies for construction work these days that the hand-over of the laboratories back to science is almost every time in time and within the scheduled finance budget. Great work!

Institute excursion Beelitzer Heilstätten

The Technical Services also organized our IKZ institute excursion on 9th September 2019 to "Beelitzer Heilstätten" in Brandenburg. On that day, one of the major rain fields of the year 2019 passed over Brandenburg which even resulted in traffic failures on the German railway system. Despite all, due to perfect organization, we had a very entertaining & interesting tour on the history of the impressive building system with a perfect barbecue under the roofs of some tents.

Alte Chirurgie in den Beelitzer Heilstätten
Old surgery in the Beelitz sanatoriums

Enjoy an inspiring lecture of IKZ´s Annual Report 2019. In case of questions, feel free to contact us and we will be happy to answer your questions.

With best regards
Thomas Schroeder

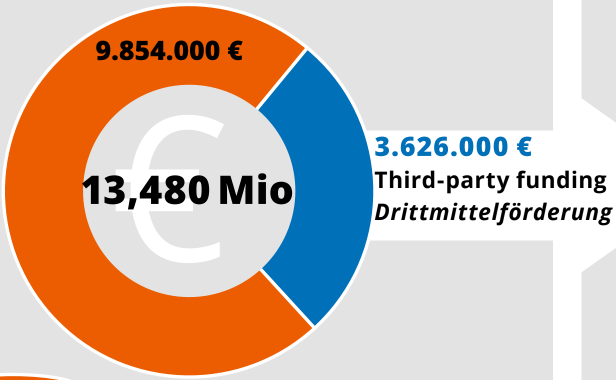
The Institute

2019 in Zahlen
2019 in figures

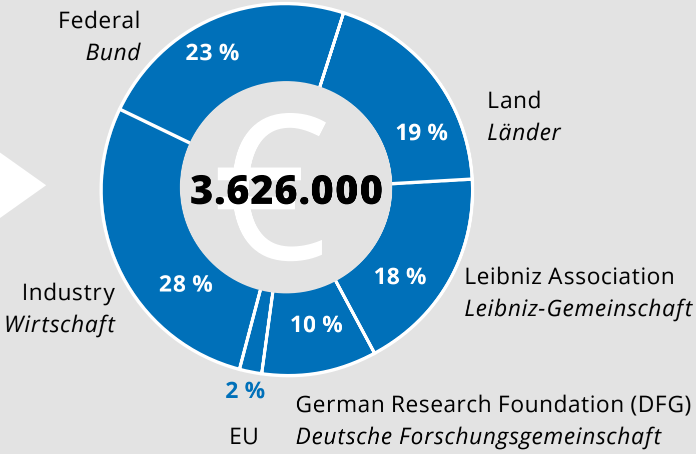
Budget

Gesamt
Total

Institutional funding
Institutionelle Förderung



Drittmittelförderung
Third-party funding



Lehre
Education

5
Abgeschlossene Promotionsarbeiten
Defended doctoral theses

19
Laufende Promotionsvorhaben
Ongoing dissertations (31.12.2019)

Publikationen
Publications

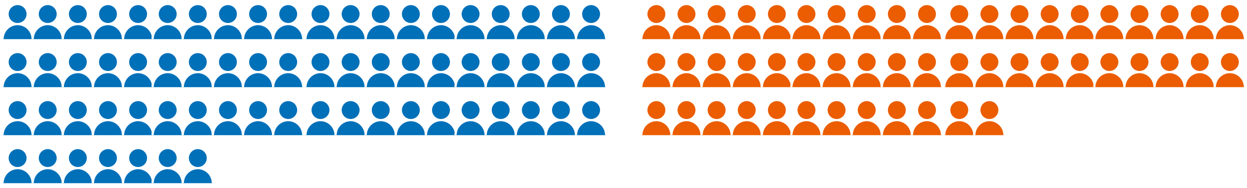
84
Artikel in referierten (peer-review) Journalen

Articles in peer-reviewed journals

Stichtag 31.12.2019

Personal gesamt
Staff total*

119

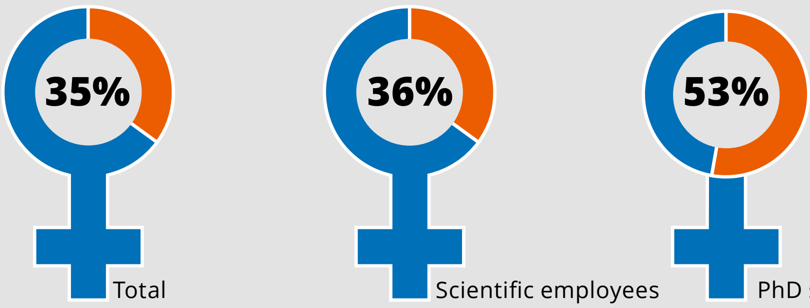


67 Scientific employees
Wissenschaftliche Mitarbeiter/innen

52 Infrastructure personnel
Infrastrukturpersonal

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

Frauenanteil
Female proportion

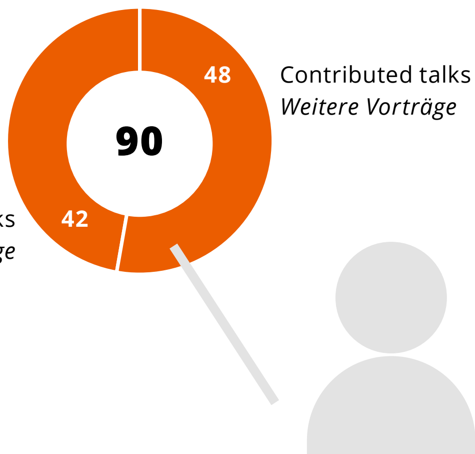


Total
Gesamt

Scientific employees
Wissenschaftliche Mitarbeiterinnen

PhD students
Doktorandinnen

Beiträge auf internationalen Konferenzen
Contributions in international conferences



Contributed talks
Weitere Vorträge

Invited talks
Eingeladene Vorträge

Veranstaltungen
Events

Kleine Forscherinnen ganz groß beim Girls' Day 2019 am IKZ

Für einen Tag in die Wunderwelt der Kristalle eintauchen. Das machten sich 10 junge Mädchen zum Ziel und verbrachten am 28.03.2019 einen spannenden Tag am IKZ. Die kleinen Forscherinnen von morgen lernten im Rahmen des Girls´Days wie Kristalle sie in ihrem alltäglichen Leben begleiten und dass unsere moderne, digitale Welt ohne Kristalle schlichtweg nicht funktionieren würde. Es wurden fleißig kleine Kristalle selbst gezüchtet und unter dem Mikroskop angeschaut. Wie das Ganze dann in groß aussieht, konnten die kleinen Forscherinnen anschließend in unseren Züchtungshallen erleben.

Young female researchers on the big stage at Girls' Day 2019 at the IKZ

Immerse yourself for a day in the wonderful world of crystals. This is what 10 young girls made their goal and spent an exciting day at the IKZ on 28.03.2019. During the Girls' Day, the little researchers of tomorrow learned how crystals accompany them in their everyday lives and that our modern, digital world would simply not function without crystals. They diligently grew small crystals themselves and looked at them under the microscope. Afterwards, the little researchers were able to experience how the whole thing looks like in large size in our growing halls.

The Institute

IKZ Sommerschule 2019

Mit dem Thema „Quantum Computing as a material Challenge" wagte sich das IKZ in diesem Jahr, unter der Leitung von Dr. Torsten Boeck, Leiter der Abteilung Schichten und Nanostrukturen, an ein völlig neues Feld heran. Dr. Lars Schreiber, Institut für Quanteninformation der RWTH Aachen, brachte den Gästen vom 2. bis 3. September 2019, neben der allgemeinverständlichen Erklärung wichtiger Prinzipien des Quantencomutings, vor allem die materialwissenschaftlichen Herausforderungen für den Bau siliziumbasierter Qubits näher.

IKZ Summer School 2019

With the topic „Quantum Computing as a material Challenge", the IKZ ventured into a completely new field this year, under the direction of Dr. Torsten Boeck, head of the department Layers and Nanostructures. From September 2nd to 3rd, 2019, Dr. Lars Schreiber (Institute for Quantum Information at RWTH Aachen University) introduced the guests to the generally understandable explanation of important principles of quantum computing. In addition, the material science challenges for the construction of silicon-based qubits were also explained.

IKZ Winterschule 2019

Vom 9.-13. Dezember 2019 hielt Prof. Dr. Peter Rudolph eine IKZ Winterschule zum Thema: „Internationale Vorlesungen zur Kristallzüchtung – Methoden, Thermodynamik, Kinetik, Transport, Defekte". Vor internationalem Publikum mit Interessierten aus insgesamt 11 Ländern erläuterte der Spezialist für Kristallisationsprozesse und Kristallzüchtungstechnologien (Crystal Technology Consulting) die ganze Bandbreite der Grundlagen der Kristallzüchtung sowie der damit verbundenen Defekterzeugung. Seine Vorträge wurden bereits in mehr als 20 Ländern auf der ganzen Welt gehalten.

IKZ Winter School 2019

From December 9-13, 2019, Prof. Dr. Peter Rudolph held an IKZ Winter School on the topic: „International Lectures on Crystal Growth - Methods, Thermodynamics, Kinetics, Transport, Defects". In front of an international audience with interested parties from a total of 11 countries, the specialist for crystallization processes and crystal growth technologies (Crystal Technology Consulting) explained the whole range of the fundamentals of crystal growth as well as the associated defect generation. His presentations have already been held in more than 20 countries around the world.

German-Polish Conference on Crystal Growth

Die 3rd German-Polish conference on Crystal Growth (GPCCG-3) wurde vom 17.-21. März 2019 in Poznań abgehalten. Die Veranstaltung stand unter der Schirmherrschaft der Polnischen Gesellschaft für Kristallzüchtung (PSCG) und der Deutschen Gesellschaft für Kristallwachstum und Kristallzüchtung (DGKK) und wurde gemeinsam von der Fakultät für Technische Physik der Technischen Universität Poznan und dem IKZ organisiert. Die enge deutsch-polnische Verbundenheit wurde unterstrichen durch die Teilnahme und Eröffnung der Konferenz durch Gabriele Harmani, Science Councellor an der Deutschen Botschaft in Polen.

Die Vorträge umfassten aktuelle und aufkommende Themen der Kristallzüchtung: Biokristalle, Lasermaterialien, Dielektrika & Intermetallika, Halbleiter, Charakterisierung und Simulation. In einer außerordentlichen Sitzung stellte der Dekan Prof. Ryszard Czajka die Forschungsaktivitäten der Fakultät für Technische Physik vor, sowie der Direktor des IKZ, Prof. Thomas Schröder, die Forschung und die neue Strategie des IKZ. In diesem Rahmen wurde auch der DGKK-Preis für die beste Doktorarbeit gemeinsam an Dr. Pascual Puphal (PSI, Villingen, Schweiz) und an Dr. Dirk Kok vergeben, der seine Arbeit am IKZ durchgeführt hatte.

German-Polish Conference on Crystal Growth

The 3rd German-Polish conference on Crystal Growth (GPCCG-3) took place in Poznań on March 17-21, 2019. The conference was held under the auspices of the Polish Society for Crystal Growth (PSCG) and the German Society for Crystal Growth (DGKK) and was jointly organized by the Faculty of Technical Physics of the Poznan University of Technology and IKZ. The close German-Polish relationship was underlined by the presence and welcome address of Gabriele Hermani, the Science Councellor of the German Embassy in Warszawa.

The talks covered relevant and emerging subjects in crystal growth: biocrystals, laser materials, dielectrics & intermetallics, nanocrystals, novel materials, semiconductors, characterization and simulation. In a special & award session the research at the Faculty of Technical Physics in Poznan was presented by its dean Prof. Ryszard Czajka and the director of IKZ, Prof. Thomas Schröder, presented the research and new strategy of IKZ. In this frame, the DGKK award for the best PhD thesis was given Dr. Pascual Puphal (PSI, Villingen, Switzerland) and Dr. Dirk Kok, who had conducted his doctorate at the IKZ.

International Conference on Silicon and Novel Semiconductor Materials

Die durch das 46th Research Institute der China Electronics Technology Group Corporation (CETC46 Institut) organisierte Konferenz fand vom 13.-15. November in Tianjin, China statt. Das CETC46 ist eines der ersten Institute in China, das sich mit der Forschung zu Halbleitermaterialien befasste und das führende chinesische Institut für Halbleitermaterialien (Si, Ge, GaAs,...), speziellen optischen Fasern und anderen funktionalen elektronischen Materialien, inklusive der neuartigen 2D-Materialien.

Die Förderung des gegenseitigen Austauschs und der Kooperation war ein zentrales Ziel der Konferenz, die sich fachlich auf die Kristallzüchtung, Simulation und Charakterisierung fokussierte. Das IKZ war mit mehreren Beiträgen vertreten: Kristallzüchtung als Schlüsseltechnologie für disruptive Technologien (Prof. Dr. Thomas Schröder), Modellierung der Floating Zone Züchtung von Silizium mit großen Durchmessern (Dr. Robert Menzel), homoepitaktisches Wachstum von β-Ga_2O_3 (Dr. Andreas Popp) und neuen Perspektiven des 2D Layer-Transfers (Dr. Jens Martin).

Um die bestehende Zusammenarbeit zwischen dem IKZ und dem CETC46 zu stärken, unterzeichneten die Institute ein Memorandum of Understanding.

International Conference on Silicon and Novel Semiconductor Materials

The conference took place on 13-15 November 2019 in Tianjin, China and had been organized by the 46th Research Institute of China Electronics Technology Group Corporation (CETC46 institute). It is one of the earliest research institutes engaged in semiconductor materials research in China and the leading Chinese research institute in semiconductor materials (Si, Ge, GaAs...), special optical fibres, and other electronic functional materials, including the recently discovered 2D-materials.

The conference aimed to promote mutual exchange and cooperation, covering topics on crystal growth, simulation technology, and characterization techniques. IKZ contributed several oral presentations covering the topics “crystals as key enabling materials for disruptive technologies”, Prof. Dr. Thomas Schröder, “Modelling of FZ growth of large diameter Si”, Dr. Robert Menzel, “homo-epitaxial growth of β-Ga_2O_3”, Dr. Andreas Popp, and “new perspectives of 2D-layer transfer”, Dr. Jens Martin.

To strengthen existing collaborations between IKZ and CETC46, the institutes signed a Memorandum of Understanding.

Nachwuchs
Young talents

PhD meets Industry, Politics and Science Administration

PhD meets Industry, Politics and Science Administration lautete das Motto des diesjährigen IKZ Doktorand*innen-Events. Auslöser war das Ergebnis einer Umfrage der Leibniz-Gemeinschaft: Viele der Promotionsstudent*innen wissen nicht, wie es nach der Promotion weitergehen soll. Welche möglichen Karrierewege gibt es? Welche Erwartungen stellt ein Arbeitgeber an einen Mitarbeiter mit Promotion? Um eine Hilfestellung bei der Beantwortung dieser existenziellen Fragen zu leisten, war es Ziel des diesjährige Events, unsere Doktorand*innen mit Alumni, Partner und Experten aus dem arbeitsnahen Umfeld des IKZ zusammenbringen. Hierbei stand der interaktive Austausch mit den eingeladenen Gästen im Fokus, da diese sich bereits in einer ähnlichen Situation befunden hatten und mittlerweile auf erfolgreiche Karrieren zurückblicken können.

In lockerer Atmosphäre sollten Erfahrungen vermittelt, Kontakte geknüpft und über Möglichkeiten gesprochen werden. Um dem einen Rahmen zu geben, wurden die Gäste in einer ersten Kennenlernrunde gebeten, ihren Karriereweg, ihre Position und ggf. ihren aktuellen Arbeitgeber kurz vorzustellen. Hierbei wurde ein Fokus auf die Hauptbeschäftigungsgebiete von promovierten Naturwissenschaftler*innen und Ingenieur*innen gelegt: Industrie, Politik und Wissenschaftsverwaltung. Anschließend gab es beim abendlichen Grillen die Möglichkeit mit den Teilnehmer*innen ins Gespräch zu kommen und persönliche Fragen zu stellen oder Ansichten auszutauschen. Das große Netzwerk des IKZ und die im selben Zeitraum stattfindenden Beiratstagung ermöglichte es, einen Einblick in Karrieren vieler verschiedener Bereiche sowie in spannende Lebensläufe erhalten.

Die Resonanz zu dem Event fiel sowohl von Seiten unserer Gäste als auch von den Doktorand*innen sehr positiv aus. Die Vielfalt der Karrieren und die Offenheit aller Teilnehmer machten die Veranstaltung zu einem voller Erfolg und gaben uns Promotionsstudent*innen einen guten Einblick in das, was da kommt – nach der Doktorarbeit.

PhD meets Industry, Politics and Science Administration

PhD meets Industry, Politics and Science Administration was the motto of this year's IKZ doctoral student event. The idea was raised by the result of a survey conducted by the Leibniz Association: many of the doctoral students do not have a clear idea of what they want to do after their doctorate. What are the possible career paths? What expectations does an employer have of an employee with a doctorate? In order to help answer these fundamental questions, the aim of this year's event was to bring our doctoral students together with alumni, partners and experts from the network of the IKZ. The event aimed for an interactive exchange with the invited guests, as they had already been in a similar situation and can now look back on successful careers.

In a relaxed atmosphere, experiences should be shared, contacts established and opportunities discussed. In order to provide a platform for this, the guests were asked to briefly present their career path, their position and, if applicable, their current employer. The focus was on the main fields of employment for material scientists and engineers with a doctorate: industry, politics and science administration. Afterwards the participants had the opportunity to talk to each other and ask personal questions or exchange views during the evening barbecue. The large network of the IKZ and the advisory board meeting, which took place on the same day, made it possible to get an insight into careers in many fields of science and engineering.

The response to the event was very positive both from our guests and from the PhD students. The diversity of careers and the openness of all participants made the event a complete success and gave us doctoral students a good insight into what's coming - after the doctorate.

Erfolgreiche Ausbildung

Neben der wissenschaftlichen Ausbildung von insgesamt 19 Promovierenden in 2019 bietet das IKZ auch die Ausbildung in verschiedenen Berufen an. 2019 schloss Alyssa Riemke ihre Ausbildung zur Kauffrau für Büromanagement erfolgreich ab, ebenso wie Tom Harbach seine Ausbildung zum Fachinformatiker für Systemintegration. Ein Zerspanungsmechaniker befindet sich noch in der Ausbildung in Zusammenarbeit mit dem ABB Ausbildungszentrum Berlin.

Successful apprenticeship

The IKZ is dedicated to the education and qualification of young people. 19 doctoral students had been performing research in the institute during the last year, and in addition the IKZ also offers professional training. In 2019, Alyssa Riemke successfully completed her training as an office management assistant, as did Tom Harbach as an IT specialist for system integration. A cutting machine operator is still completing his training in cooperation with the ABB Training Center Berlin.

The Institute

Auszeichnungen
Awards

Prof. Darrell Schlom, Cornell University (USA) und Dr. Reinhard Uecker, Leibniz-Institut für Kristallzüchtung (IKZ, Deutschland) erhielten gemeinsam den Frank-Preis der Internationalen Organisation für Kristallzüchtung (IOCG) für ihre „bahnbrechenden Beiträge zur Entwicklung neuer Perowskit-Substrate, die ein strain engineering funktioneller Oxide ermöglichen".

For their "pioneering contributions to the development of new perovskite substrates enabling strain engineering of functional oxides", Prof. Darrell Schlom, Cornell University (USA) and Dr. Reinhard Uecker, Leibniz-Institut für Kristallzüchtung (IKZ, Germany) were jointly awarded the Frank Prize by the International Organization for Crystal Growth (IOCG).

Prof. Darrell Schlom

Dr. Reinhard Uecker

"A thin film is only as good as its substrate"

ein Interview mit / an interview with Prof. Dr. Darrell G. Schlom

Der Frank-Preis ist die höchste Auszeichnung der IOCG und wird höchstens einmal alle drei Jahre verliehen. Dieser Preis wird für herausragende, grundlegende Beiträge auf dem Gebiet der Kristallzüchtung durch technische Errungenschaften, Veröffentlichungen und Präsentationen sowie durch einen weltweiten Beitrag zu Wissenschaft und Technik verliehen. Der Preis wurde nach einer gemeinsamen Präsentation der Preisträger während der Internationalen Konferenz über Kristallzüchtung und Epitaxie ICCGE-19, die vom 28. Juli bis 2. August in Keystone, Colorado, stattfand, verliehen.

„Die Basis der oxidischen Schicht ist das Substrat und demnach besonders wichtig! Deshalb bin ich überhaupt hier am IKZ." sagt Experte für Epitaxie, Darrell Schlom. Er weist darauf hin, dass er eigentlich kein „echter" Kristallzüchter ist. Darrells Forschungsgebiet behandelt die Eigenschaften von Oxidmaterialien für die Elektronik. Zu diesem Zweck züchtet er dünne Oxidschichten auf einkristallinen Substraten aus eng verwandten kristallinen Materialien.

The Frank Prize is the highest prize of the IOCG and is given at most once every three years. This prize is for outstanding, fundamental contributions to the field of crystal growth through technical achievements, publications and presentations, and through its global contribution to science and technology. The award was presented following a joint presentation by the award winners during the International Conference on Crystal Growth and Epitaxy ICCGE-19, which was held in Keystone, Colorado from July 28 to August 2.

"A thin film is only as good as its substrate and that is precisely why I came to IKZ for sabbatical" says expert for epitaxy **Darrell Schlom**. He points out that he is not a „real" crystal grower. Darrell's research field is on the properties of oxide materials for electronics. For that purpose he grows thin oxide layers on single crystalline substrates of closely related materials.

Können Sie uns sagen, wie diese langjährige Zusammenarbeit begann?

Darrell Schlom: *1996 auf der ACCG-10 Konferenz in Vail, Colorado, habe ich Dr. Reinhard Uecker und Dr. Peter Reiche vom IKZ kennengelernt, die ebenso an oxidischen Schichten gearbeitet haben. Eine länderübergreifende Zusammenarbeit der Bereiche „Volumenkristalle" und „Schichten" ist eher ungewöhnlich. Genau das war aber das Interessante daran und so sind bis heute 35 gemeinsame Publikationen aus dieser intensiven Zusammenarbeit zwischen dem IKZ und mir hervorgegangen. Ich bin immer wieder auf der Suche nach neuen Substraten. Nur so kann ich auch gute Schichten hervorbringen. Insgesamt haben wir im Laufe unserer Zusammenarbeit 20 Materialien gemeinsam untersucht.*

Sie sind ein perfektes Beispiel, um zu zeigen, wie wichtig eine gute Zusammenarbeit ist. Aber warum forschen so wenige US-Wissenschaftler in Deutschland auf diesem Gebiet?

Das verstehe ich auch nicht. Die Wissenschaftler verpassen eine gute Chance. Auf der anderen Seite treffe ich immer wieder Wissenschaftler, die sehr an einer Zusammenarbeit mit anderen Instituten interessiert sind. Sowohl die Zusammenarbeit mit Europa also auch mit Asien ist besonders wichtig für die USA. In unserem Land legen wir den Fokus eher auf die Anwendungen. Das finde ich sehr schade. Meiner Meinung nach sollte jeder auch Grundlagenforschung betreiben. Auf der anderen Seite merken die Menschen hier aber auch, dass es von Vorteil ist, neue Materialien zu finden. Ein gutes Beispiel hierfür ist Graphen (was aus Europa kommt): Das ist bislang in Nordamerika eher schleppend angekommen.

Vielleicht sollten wir unsere Sichtbarkeit in den USA erhöhen?

Ja, absolut. Die Leute sind grundsätzlich daran interessiert. Ich werde immer wieder nach Möglichkeiten gefragt, wo und wie eine Zusammenarbeit mit deutschen Instituten im Bereich der Epitaxie möglich wäre.

Can you tell us how this long lasting cooperation began?

Darrell Schlom: *It was in 1996 at the ACCG-10 Conference in Vail, Colorado that I first met Dr. Reinhard Uecker and Dr. Peter Reiche from IKZ. We shared an interest in the growth of oxide crystals, albeit from different perspectives. Their expertise was in bulk crystal growth and mine the growth of thin films. From their work it was clear that they were making oxide crystals of exceptional quality. I am always on the lookout for new substrates as only with good substrates is it possible to grow good thin films. It is a bit unusual for thin film growers to collaborate with bulk crystal growers, but so began our long lasting international collaboration that has produced more than 35 joint publications to date. The superb oxide single crystals from IKZ have enabled us to prepare and jointly study over 20 different materials in thin-film form. These films have enhanced properties that arise from the strain engineering imposed by the underlying substrates.*

You are a perfect example to show the importance of a good cooperation. But why are there so few scientists from the USA doing research in Germany in this area?

I also don't understand why. Other scientists are missing a great opportunity! Back in the U.S.A. I am constantly meeting scientists interested in establishing international collaborations. Perhaps the reason that more are not working and collaborating in this area is that in our country there is a stronger focus on applications and less appreciation that it often takes years of fundamental research to lay the foundation for applications. In my opinion, every scientist should also have the opportunity to be involved in some fundamental research. Discovering new materials is crucial to new applications. Graphene, for which the discovery was made in Europe, is an excellent example in this regard. I am hopeful that this and other examples will help increase the appreciation in the U.S.A. for fundamental research, especially involving the discovery and perfecting of new materials.

Maybe we should enhance our visibility in the USA?

Absolutely! People are basically interested. I am often asked how it is possible to establish a collaboration with German institutes in the area of epitaxy.

The Institute

Sie arbeiten seit mehr als zwei Jahrzehnten mit dem IKZ zusammen. Haben Sie irgendwelche Empfehlungen für das Institut?

Noch mehr Brücken zu bauen! Es gibt allein in Deutschland so viele Möglichkeiten. Man sollte nicht versuchen alles selber zu machen, sondern lieber seinen Kern nicht verlieren und vielmehr eine intensive Zusammenarbeit anstreben. Nur so kann man die Konzentration von einem Material weglenken und sich mit Substraten beschäftigen, die die Wissenschaft interessiert und die Zukunft haben. Aber ich bin überzeugt davon, dass das IKZ auf einem guten Weg ist. Aus den Ländern müssen neue Technologien kommen. Das ist nur mit einer Zusammenarbeit zwischen den Ländern möglich. Nur so kann man neue Verbindungen mit besseren Eigenschaften hervorbringen.

Darrell Schlom ist der Herbert Fisk Johnson-Professor für industrielle Chemie in der Abteilung für Materialwissenschaften und Ingenieurwesen an der Cornell University in Ithaca, USA. Er erhielt die MRS-Medaille der Materials Research Society und einen Humboldt-Forschungspreis; er ist Fellow der American Physical Society, der American Vacuum Society und der Materials Research Society und ist Mitglied der National Academy of Engineering der USA.

Seit mehr als 20 Jahren arbeitet Darrell Schlom eng mit dem IKZ zusammen. Im Jahr 2019 gab ihm der Humboldt-Forschungspreis die Gelegenheit zu einem mehrmonatigen Forschungsaufenthalt am Institut, um gemeinsam mit dem IKZ-Wissenschaftler Dr. Christo Guguschev neue Substrate zu erforschen.

You have been cooperating with IKZ for more than two decades. Do you have any recommendations for the institute?

My advice is to build more bridges! In Germany alone there are so many possibilities for enhanced collaborations that would extend and enhance IKZ's impact. One should not try to do everything in-house. It is far better to strengthen one's core competency and forge strategic collaborations with outside institutions that can provide needed competencies quickly and with high quality. The external competencies that IKZ needs will change over time. A benefit of having and continuing to advance its world-leading core competency in crystal growth is that IKZ can be nimble and selective in the partnerships that it makes. Through such strategic bridge building it will be possible for IKZ to continue to discover and perfect better crystals. By partnering IKZ can enable the application potential of each of these new materials to be pursued. The attraction of outside collaborators to IKZ is the high-quality crystals in its portfolio, crystals that are the enablers to new and improved technologies. I am convinced that IKZ is on the right track.

Darrell Schlom is the Herbert Fisk Johnson professor of industrial chemistry in the department of Materials Science and Engineering at Cornell University in Ithaca, USA. He received the MRS Medal from the Materials Research Society and a Humboldt Research Award; he is a Fellow of the American Physical Society, the American Vacuum Society, and the Materials Research Society, and is a member of the National Academy of Engineering of U.S.A.

For more than 20 years Darrell Schlom has been working in close cooperation with the IKZ. In 2019, the Humboldt Research Award gave him the opportunity to spend several months for another research stay at the institute to research new substrates in cooperation with IKZ scientist Dr. Christo Gugushev.

Nachwuchspreis DGKK

Dr. Dirk Johannes Kok wurde für seine Forschungen über den Einfluss der Wachstumsbedingungen auf die optischen Eigenschaften von Strontiumtitanat mit dem Nachwuchspreis der Deutschen Gesellschaft für Kristallwachstum und Kristallzüchtung ausgezeichnet. Im Rahmen seiner Dissertation am Leibniz-Institut für Kristallzüchtung erforschte er anwendungsrelevante Zusammenhänge zwischen der Wachstumsatmosphäre, der Stöchiometrieabweichung im Kristall und der damit verbundenen Änderung des Gitterparameters. Seine Beobachtungen zum Verlauf der temperaturabhängigen Wärmeleitfähigkeit und Bandlücke sind auf viele andere komplexe Oxidmaterialien anwendbar.

DGKK Young Scientist Award

Dr. Dirk Johannes Kok has been awarded by the German Association for Crystal Growth (DGKK) for his PhD thesis on the growth and optical properties of strontium titanate. In the frame of his thesis at the Leibniz-Institut für Kristallzüchtung he researched on models for application-relevant correlations between the growth atmosphere, the stoichiometric deviation in the crystal and the associated change of the lattice parameter. His results on the temperature-dependent thermal conductivity and band gap are applicable to many other complex oxide materials.

Ausgewählte Projekte
Featured Projects

Erfolgreicher Start des Zentrums für Lasermaterialen am IKZ

In der Materialbearbeitung, der Medizin oder der Metrologie – Laser sind allgegenwärtig in unserem täglichen Leben. Auch 60 Jahre nach dieser bahnbrechenden Erfindung ist die Forschung an neuen Lasermaterialien mit verbesserten Eigenschaften noch ein hochaktuelles Forschungsthema. Gesucht werden Materialien für neue Wellenlängenbereiche im ultravioletten (UV) oder mittleren infraroten Spektralbereich, aber selbst im sichtbaren gibt es noch Bereiche, die nur mit komplexen und teuren Lasersystemen erreichbar sind. Auch höhere Ausgangsleistungen bzw. kürzere Pulsdauern sind gefragt, um die einzigartigen Eigenschaften dieser kohärenten Lichtquellen voll ausnutzen zu können.

Um die Materialforschung in diesem Bereich voranzutreiben, starteten das Leibniz-Institut für Kristallzüchtung (IKZ) und das Ferdinand-Braun-Institut (FBH) vor einigen Jahren eine gemeinsame Initiative. Im August 2016 wurde das BMBF-Projekt „EQuiLa" zur Erforschung und Qualifizierung innovativer Lasermaterialien und Kristalle eingeworben. Die Fördermittel ermöglichten die Einrichtung neuer Labore für das Zentrum für Lasermaterialien – Kristalle (ZLM-K) am IKZ sowie das Zentrum für Lasermaterialien – Halbleiter (ZLM-H) am FBH. Die Forschung am ZLM-H ist der Erforschung und Herstellung von Halbleiter-Lasermaterialien gewidmet, während der Fokus der Arbeiten am ZLM-K der Untersuchung kristalliner Materialien für Festkörperlaser gilt.

Dr. Christian Kränkel, Leiter des ZLM-K, erläutert das Konzept: „Die Forschung am ZLM deckt die gesamte Wertschöpfungskette von diodengepumpten Festkörperlasern von der Züchtung der Laserkristalle und deren Präparation über die Züchtung der Halbleiterstrukturen und den Bau von Diodenlasern bis zum Aufbau von Laserdemonstratoren ab. Unser Ziel ist es, die europaweit führende Anlaufstelle für alle Fragen bezüglich Lasermaterialien zu werden." Eine kürzlich von Felix Mauerhoff eingereichte Abschlussarbeit zu einem mit einem roten Diodenlaser gepumpten Chrom-dotierten $LiCAlF_6$-Laser ist ein gelungener Beleg für dieses Konzept: Alle Schlüsselkomponenten für diesen Laser wurden am ZLM hergestellt, die Laserkristalle wurden am IKZ gezüchtet und die roten Pumpdioden stammen aus dem FBH.

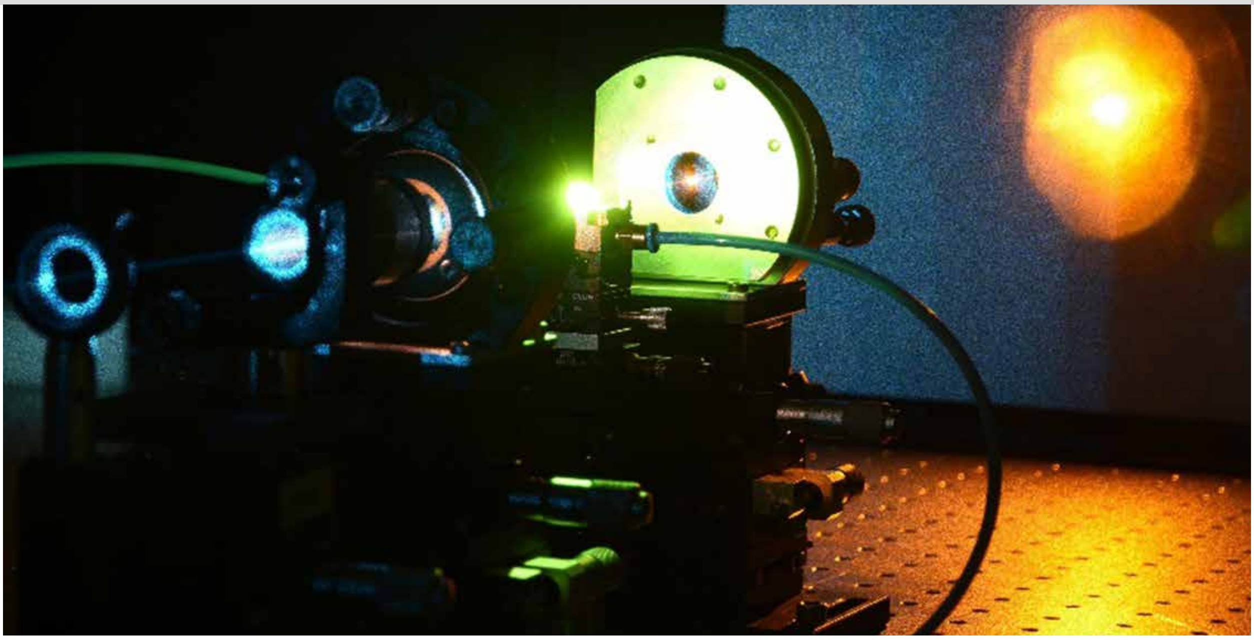
Center for Laser Materials successfully established at the IKZ

In materials processing, medicine or in metrology – lasers are ubiquitous in daily life. Even 60 years after this groundbreaking invention, the quest for active laser materials with improved properties is topical. Current research is heading for laser sources covering new wavelength regions in the ultraviolet (UV) or mid-infrared (mid-IR) spectral range, but even in the visible range there are still gaps which cannot directly be addressed by practical systems. Researchers are also aiming for ever higher output power and/or shorter pulse durations to make best use of the unique properties of coherent light radiation.

To find a remedy in all materials related questions in this research area, the Leibniz-Institut für Kristallzüchtung (IKZ) and the Ferdinand-Braun-Institut (FBH) started a common initiative. In August 2016 the BMBF-project "EQuiLa" on the research and qualification of innovative laser materials and crystals was granted. The funding within this project enabled installing new laboratories for the Center for Laser Materials – Crystals (ZLM-K) at the IKZ and the Center for Laser Materials – Semiconductors (ZLM-H) at the FBH since then. The research at the ZLM-H is devoted to the development and growth of semiconductor laser materials, the main focus of the research at the ZLM-K is the investigation of crystalline laser gain media.

Dr. Christian Kränkel, leader of the ZLM-K, elucidates the concept: "The research at the ZLM covers the whole value chain of diode-pumped solid-state lasers starting from the growth of laser crystals and their polishing over the growth of semiconductor-films for laser diodes and their packaging and ending with setting up laser demonstrators. We aim to be the leading European one-stop-agency for all laser material related questions". A recent thesis of Felix Mauerhoff on red-diode-pumped Cr-doped $LiCaAlF_6$ lasers nicely illustrates this concept: All key components for his laser were fabricated at the ZLM, the laser crystals were grown at IKZ and the high power red pump diodes were fabricated at FBH.

The Institute



Der weltweit erste diodengepumpte Terbium-Laser
The world's first diode-pumped terbium-laser

Die Kompetenzen am ZLM-K decken die Entwicklung und Züchtung neuer Lasermaterialien ab, sowie die die hochgenaue Bestimmung laserrelevanter spektroskopischer Parameter und natürlich die Charakterisierung beim Einsatz als aktive Materialien in Festkörperlasern. Die hierfür benötigte experimentelle Ausstattung umfasst u.a. verschiedene moderne Züchtungsöfen für die Züchtung von Laserkristallen, die in enger Abstimmung mit der Sektion „Oxide & Fluoride" am IKZ ausgewählt und aufgebaut wurden. Eine neue Czochralski-Anlage ermöglicht die Züchtung von Oxidmaterialien aus Iridium-Tiegeln bei Temperaturen bis zu 2200 °C, was die wichtigsten Lasermaterialien wie z.B. Seltenerd-dotierte Granatkristalle mit einschließt. Zusätzlich wurden zwei Anlagen zum optischen Zonenschmelzen (engl. *Optical Floating Zone (OFZ))* beschafft. Dieses tiegelfreie Züchtungsverfahren hat den großen Vorteil, dass die Züchtungsatmosphäre frei gewählt werden kann, ohne dass es zu Reaktionen mit dem Tiegelmaterial kommt. Zudem gestattet eine dieser Anlagen Kristallzüchtung bis zu Temperaturen von bis zu 3000 °C und ermöglicht damit beispielsweise die Züchtung hochschmelzender Sesquioxide, die geeignet sein könnten, einige der gegenwärtigen Herausforderungen in der Laserforschung zu lösen. Die erfolgreiche Züchtung von Erbium-dotiertem Lutetiumoxid [1] ist der erste Beleg für den Erfolg dieses Forschungsansatzes. Die Kristallzüchterin Anastasia Uvarova, Doktorandin am ZLM-K freut sich über diesen Erfolg: „Dieser ansonsten schwer zu züchtende Kristall ist wichtig für Laser im mittleren infraroten Spektralbereich, die z.B. für Laserskalpelle in der Medizin benötigt werden." Die Aktivitäten im Bereich der Züchtung von Laserkristallen wurden weiter gestärkt durch die Einrichtung einer Nachwuchsgruppe unter der Leitung von Dr. Hiroki Tanaka zum Thema „Fluorid-Kristalle für photonische Anwendungen". Die interdisziplinäre Forschung von Dr. Tanaka zielt darauf ab, die Zusammenarbeit mit der Sektion „Oxide & Fluoride" hinsichtlich anwendungsspezifischer Kristalle für Laser und andere photonische Anwendungen auf ein neues Niveau zu heben.

The competences at the ZLM-K cover the conception and growth of novel laser materials as well as detailed laser relevant spectroscopic investigation capabilities for ion-doped crystals and of course their characterization in solid-state laser resonators. The equipment acquired for these tasks includes different state-of-the-art furnaces for the growth of laser crystals, set up in close collaboration with researchers from the Oxide & Fluoride growth section at IKZ. A new Czochralski growth furnace enables the growth of oxide laser crystals from iridium crucibles at temperatures up to 2200 °C, including typical laser materials such as rare-earth doped garnets. In addition, two optical floating zone (OFZ) growth furnaces were acquired. This technique is crucible free, which is a huge advantage as it allows for a large variety of growth atmospheres and high temperatures without any detrimental influence on the crucible material. One of these OFZ furnaces sustains growth temperatures of up to 3000 °C, allowing for the growth of highly melting sesquioxides, a class of laser materials which is thought to solve some of the challenges in current laser research. The successful growth of erbium-doped lutetia [1] is a first evidence for the suitability of this approach. The crystal grower, Anastasia Uvarova, PhD-student at the ZLM-K, is happy about this result: "This difficult to grow crystal is important for mid-infrared lasers, needed for example in laser scalpels in medicine." The activities on laser crystal growth are further intensified by a new IKZ junior research group led by Dr. Hiroki Tanaka on 'fluoride crystals for photonics applications'. His interdisciplinary research aims to boost the cooperation with the Oxide & Fluoride growth section towards application-specific crystals for lasers and other photonic applications.

The Institute

Das ZLM-K ist außerdem ausgestattet für die optische Spektroskopie an Lasermaterialien mit gepulsten Anregungsquellen im Wellenlängenbereich von 205 nm im UV bis zu 2,4 µm im mittleren Infraroten wie auch mit leistungsstarken spektral durchstimmbaren Dauerstrichquellen im Wellenlängenbereich zwischen 350 nm und 1000 nm. Im Zusammenspiel mit modernen Detektoren erlaubt diese Ausstattung zeitaufgelöste wie auch statische Spektroskopie vom UV bis in den mittleren infraroten Spektralbereich. So wurden am ZLM in Zusammenarbeit mit der Belarusian Technical University BNTU in Minsk die optischen Eigenschaften Terbium-dotierter Wolframat-Kristalle im sichtbaren Spektralbereich ermittelt und in Zusammenarbeit mit der Universität von Pisa in Italien erstmals Praseodym-dotierte Sesquioxide im mittleren Infraroten charakterisiert [2,3]. Auch wurden bereits in einer Kooperation mit der Keio Universität in Yokohama in Japan zeitaufgelöste Messungen an sättigbaren Absorber-Kristallen zum passiven Güteschalten durchgeführt.

Schließlich ist das ZLM mit einer Vielzahl von Pumpquellen, Optomechaniken und Laserspiegeln ausgestattet, die eine Lasercharakterisierung neuer Materialien vom sichtbaren bis in den Bereich von 3 µm im Dauerstrich und gepulsten Betrieb erlaubt. Ein Beispiel hierfür ist der erste diodengepumpte Festkörperlaser basierend auf einem Tb-dotierten Laserkristall (Tb:$LiLuF_4$) [4]. „Dieser Laser stellt einen wichtigen Schritt auf dem Weg zur kommerziellen Nutzung Tb-dotierter Kristalle für gelbe Laser dar“, sagt die Laserspezialistin Elena Castellano, Doktorandin am ZLM-K.

All diese Beispiele dokumentieren den erfolgreichen Start des ZLM-K als Kompetenz-Zentrum für die Forschung und Entwicklung von Laserkristallen. Dabei sind die Aktivitäten am ZLM-K nicht nur auf die Grundlagenforschung zu Festkörperlasern beschränkt. In verschiedenen Kooperationen mit renommierten Industriepartnern werden auch neue Komponenten für kommerzielle Lasersysteme entwickelt. Das ZLM-K bietet die Charakterisierung und Qualifikation von Laserkristallen auch als Dienstleistung für Partner an Hochschulen und in der Industrie an. Um all diese Aufgaben zukünftig zu bewältigen, wird das ZLM-K im Frühjahr 2020 neue, größere Laborräume beziehen. Damit wird der Grundstein gelegt für die weitere erfolgreiche Arbeit im Bereich innovativer diodengepumpter Festkörperlaser basierend auf am IKZ gezüchteten Laserkristallen.

3The ZLM-K is also equipped for the optical spectroscopy of laser materials including pulsed ns-excitation sources at wavelengths from 205 nm in the UV up to 2.4 µm in the mid-IR as well as powerful continuous-wave (cw) excitation sources covering the range from 350 nm to 1000 nm with only few gaps in the dark red region. In combination with state-of-the-art detection, the ZLM-K is ready for time resolved and steady state optical spectroscopy from the UV to the mid-IR range. ZLM-researchers already investigated optical properties of terbium-doped tungstate crystals in the visible in cooperation with the BNTU in Belarus or those of praseodymium doped sesquioxides in the mid-IR together with the University of Pisa in Italy [2,3], but also time resolved optical characterization of saturable absorber crystals for *Q*-switching was shown in cooperation with the Keio University in Japan [4].

Finally, the ZLM is equipped with pump sources, optomechanics, and a huge variety of laser mirrors enabling laser material characterization from the visible to the 3 µm spectral range in cw and pulsed operation. As an example, ZLM-researchers demonstrated the first diode-pumped terbium-doped solid-state laser based on terbium-doped lithium-lutetium-fluoride (Tb:$LiLuF_4$) [4]. “The first application of such a simple pumping source is an important step toward the commercial use of yellow terbium-lasers”, says laser specialist Elena Castellano, PhD-student at the ZLM-K.

All this demonstrates the successful installation of the ZLM-K as a competence center for laser crystal research and development. As such, the activities of the ZLM-K are not limited to basic research. Several collaborations with renowned partners from industry have been initiated targeting the development of new components for commercial laser systems. The ZLM-K also offers laser crystal qualification as a service for partners in academia and industry. To tackle all these tasks the ZLM-K will move to new labs with increased space and resources in early 2020. This will pave the way for further successful work in the area of innovative diode-pumped solid-state lasers based on laser crystals grown at IKZ.

The Institute

C. Kränkel, E. Castellano-Hernández, S. Kalusniak,
L. Ollenburg, F. Mauerhoff, and H. Tanaka

Center for Laser Materials at the
Leibniz-Institut für Kristallzüchtung,
Berlin, Germany

[1] A. Uvarova, C. Guguschev, and C. Kränkel
Growth and characterization of high-melting sesquioxides for 3 μm lasers
Conference on Lasers and Electro-Optics (CLEO/Europe-EQEC) 2019, Munich, Germany, talk CA-10.2

[2] M. Demesh, A. Mudryi, A. Pavlyuk, E. Castellano-Hernández, C. Kränkel, and N. Kuleshov
Cross sections and transition intensities of Tb^{3+} in $KY(WO_4)_2$ OSA Continuum **2** (4), 1378-1385 (2019)

[3] A. Toncelli, J. H. Xu, A. Tredicucci, A. M. Heuer, and C. Kränkel
Mid Infrared spectroscopic characterization of Pr^{3+}:Lu_2O_3
Opt. Mat. Express **9** (11), 4464-4473 (2019)

[4] H. Tanaka, C. Kränkel, and F. Kannari
Transition-metal-doped saturable absorbers for passive Q-switching of visible lasers
Opt. Express (submitted)

[5] E. Castellano-Hernández, S. Kalusniak, P. W. Metz, and C. Kränkel
Diode-pumped laser operation of Tb^{3+}:$LiLuF_4$ in the green and yellow spectral range
Laser Photon. Rev. **14** (2), 1900229 (2020)

C. Kränkel, E. Castellano-Hernández, S. Kalusniak,
L. Ollenburg, F. Mauerhoff, and H. Tanaka

Center for Laser Materials at the
Leibniz-Institut für Kristallzüchtung,
Berlin, Germany

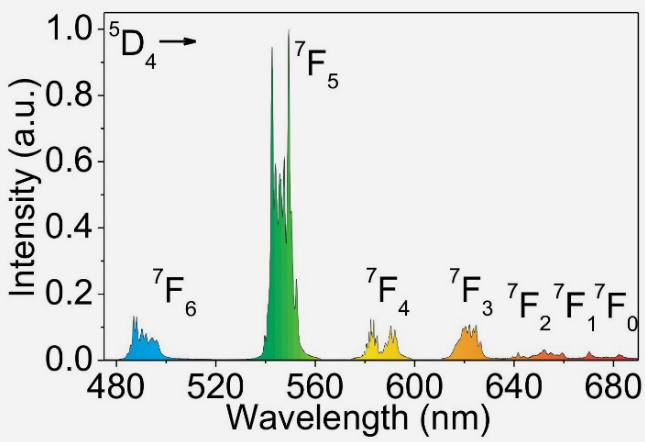
[1] A. Uvarova, C. Guguschev, and C. Kränkel
Growth and characterization of high-melting sesquioxides for 3 μm lasers
Conference on Lasers and Electro-Optics (CLEO/Europe-EQEC) 2019, Munich, Germany, talk CA-10.2

[2] M. Demesh, A. Mudryi, A. Pavlyuk, E. Castellano-Hernández, C. Kränkel, and N. Kuleshov
Cross sections and transition intensities of Tb^{3+} in $KY(WO_4)_2$ OSA Continuum **2** (4), 1378-1385 (2019)

[3] A. Toncelli, J. H. Xu, A. Tredicucci, A. M. Heuer, and C. Kränkel
Mid Infrared spectroscopic characterization of Pr^{3+}:Lu_2O_3
Opt. Mat. Express **9** (11), 4464-4473 (2019)

[4] H. Tanaka, C. Kränkel, and F. Kannari
Transition-metal-doped saturable absorbers for passive Q-switching of visible lasers
Opt. Express (submitted)

[5] E. Castellano-Hernández, S. Kalusniak, P. W. Metz, and C. Kränkel
Diode-pumped laser operation of Tb^{3+}:$LiLuF_4$ in the green and yellow spectral range
Laser Photon. Rev. **14** (2), 1900229 (2020)



Über beide Polarisationen gemittelte sichtbare Fluoreszenz von Tb:KYW
© Optical Society of America

Polarization averaged visible fluorescence of Tb:KYW
Courtesy of the Optical Society of America

IKZ-Forscher Kaspars Dadzis erhält ERC Starting Grant

Kaspars Dadzis mit einem Demo-Aufbau für Kristallzüchtung.
Kaspars Dadzis with a demo setup for crystal growth.

Erstmals in der Geschichte des IKZ wird der begehrte Starting Grant des Europäischen Forschungsrats (ERC) an einen IKZ-Forscher vergeben. Als einer von insgesamt vier Wissenschaftlern in Deutschland behauptete sich Kaspars Dadzis im Panel „Products and Processes Engineering". Für sein Projekt „Next Generation Multiphysical Models for Crystal Growth Processes (NEMOCRYS)" erhält er über einen Zeitraum von 5 Jahren insgesamt 1,5 Millionen Euro.

Kristallwachstumsprozesse sind sowohl in der Forschung als auch in der industriellen Produktion hochkomplexe physikalische Phänomene. Sogar auf einer makroskopischen Ebene sind sie mit dem Elektromagnetismus, der Strömungsmechanik und vielen anderen Bereichen der physikalischen Wissenschaft und Technik verknüpft. Häufig wird dabei die numerische Simulation zur Prozessoptimierung eingesetzt, um die Materialqualität und Prozesseffizienz zu erhöhen. Der Mangel an Möglichkeiten für direkte Messungen innerhalb von Kristallzüchtungsumgebungen schränkt jedoch die erreichbare Genauigkeit der zugrunde liegenden theoretischen Modelle ein. Folglich dominiert immer noch ein experimenteller Trial-and-Error-Ansatz die Praxis der Kristallwachstumsentwicklung. Diese Herausforderungen wird die neue Nachwuchsforschergruppe „Modellexperimente" unter der Leitung von Kaspars Dadzis in Angriff nehmen.

Das NEMOCRYS-Projekt widmet sich der Entwicklung einer neuen experimentellen Plattform, welche einzigartige Kristallzüchtungsanlagen für Modellmaterialien beinhaltet. Das zielgerichtete Design dieser Anlagen, die reduzierten Betriebstemperaturen und die geringeren Anforderungen an die Vakuumabdichtung ermöglichen einen unkomplizierten experimentellen Zugang für verschiedene in-situ-Messtechniken. Solche Modellexperimente sind in vielen Bereichen gut etabliert – vom aerodynamischen Design mithilfe von Windtunneln zur Erfdorschung des Geo-Magnetismus mithilfe von Labormodellen des Erdkerns aus flüssigem Metall.

Modellexperimente im NEMOCRYS-Projekt werden durch die gleichzeitige Beobachtung von Wärmefeldern, Strömungen, Spannungsverteilungen und anderen physikalischen Phänomenen erstmals ermöglichen, eine Reihe von grundlegenden Annahmen in multiphysikalischen makroskopischen Modellen für das Kristallwachstum zu validieren. Das Projekt hat das anspruchsvolle Ziel, eine neue Ebene des physikalischen Verständnisses zu erreichen und das Paradigma zu ändern, wie wir Kristallwachstumsprozesse und ähnliche komplexe multiphysikalische Systeme beobachten, beschreiben und entwickeln. Die praktischen Ergebnisse in Form neuer physikalischer Modelle und optimierter Messtechniken werden zur Unterstützung verschiedener Entwicklungsprojekte am IKZ eingesetzt.

Nach dem Abschluss seiner Promotion arbeitete Kaspars Dadzis in der industriellen Forschung bei SolarWorld in Freiberg mit dem Schwerpunkt Züchtung von Siliziumkristallen für Solarzellen.

Im Jahr 2016 wechselte er an das IKZ. Für seine Arbeiten auf dem Gebiet der Modellversuche und der numerischen Simulation für das Kristallwachstum erhielt er 2017 den „LIMTECH Young Scientist Award". Diese Arbeiten (siehe, z.B., [1,2]) haben das hohe Potenzial einer komplementären experimentellen und numerischen Modellierung demonstriert und dadurch die wesentliche Motivation für das NEMOCRYS-Projekt geschaffen.

[1] K. Dadzis, P. Bönisch, L. Sylla, T. Richter, Validation, verification, and benchmarking of crystal growth simulations, Journal of Crystal Growth 474 (2017) 171-177.

[2] K. Dadzis, O. Pätzold, G. Gerbeth, Model Experiments for Flow Phenomena in Crystal Growth, Crystal Research and Technology, 1900096 (2019).

IKZ researcher Kaspars Dadzis receives ERC Starting Grant

For the first time in the history of the IKZ the European Research Council (ERC) awarded the prestigious Starting Grant to an IKZ researcher. As one of a total of four scientists in Germany, Kaspars Dadzis asserted himself in the "Products and Processes Engineering" panel. For his project "Next Generation Multiphysical Models for Crystal Growth Processes (NEMOCRYS)" he will receive a total of 1.5 million euros over a period of five years.

Crystal growth processes both in research and industrial production are highly complex physical phenomena. Even on a macroscopic scale they involve electromagnetism, fluid dynamics, and many other branches of physical science and engineering. In that context numerical simulation is often used for process optimization to increase material quality and process efficiency. However, the lack of possibilities for direct measurements inside of crystal growth environments limits the achievable accuracy of the underlying theoretical models. Consequently, an experimental trial-and-error approach still dominates the practice of crystal growth development. This challenge will be addressed in the new junior research group "Model experiments" led by Kaspars Dadzis.

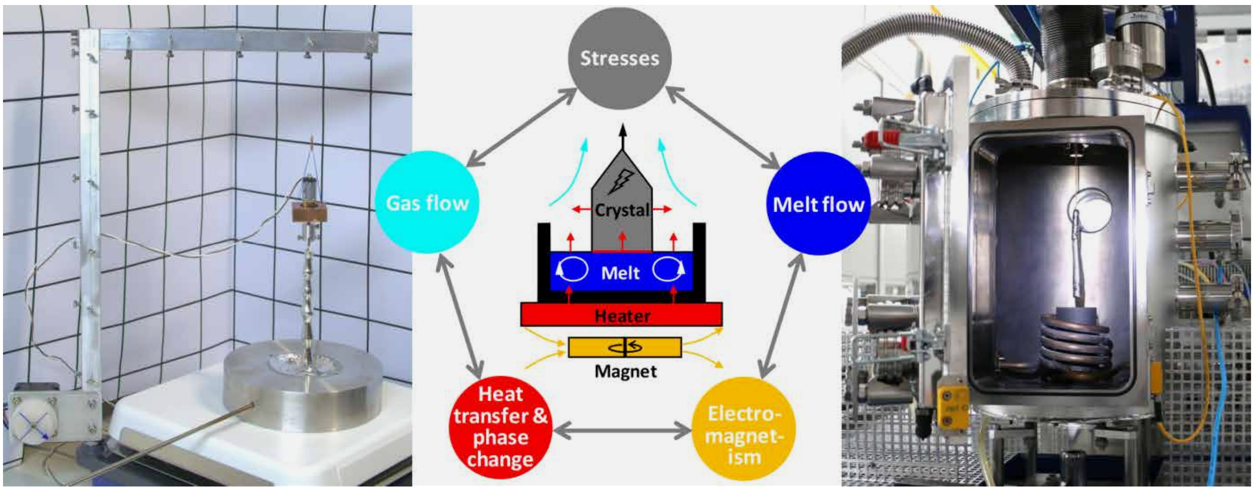
In the NEMOCRYS project a new experimental platform with unique crystal growth setups for model materials will be developed. The dedicated design of these setups, reduced working temperatures, and relaxed vacuum-sealing requirements will enable a convenient experimental access for various in-situ measurement techniques. Such model experiments are well-established in many fields – from aerodynamics design using wind tunnels to geo-magnetism research using laboratory models of Earth's liquid metal core.

Model experiments in the NEMOCRYS project with the simultaneous observation of thermal fields, fluid flows, stress distributions and other physical phenomena will allow for the first time to thoroughly validate a series of fundamental assumptions in multiphysical macroscopic models for crystal growth. The project has the ambitious goal to reach a new level of physical understanding and to change the paradigm how we observe, describe and develop crystal growth processes and similar complex multiphysical systems. The practical results in form of new physical models and optimized measurement techniques will be applied to support various development projects at the IKZ.

After the completion of his PhD thesis, Kaspars Dadzis worked in the industrial research at SolarWorld in Freiberg focusing on silicon crystal growth for solar cells. In 2016 he moved to the IKZ. He received the LIMTECH Young Scientist Award for his work in the field of model experiments and numerical simulation in crystal growth in 2017. These studies (see, e.g., [1, 2]) demonstrated the high potential of complementary experimental and numerical modeling and provided an essential motivation for the NEMOCRYS project.

[1] K. Dadzis, P. Bönisch, L. Sylla, T. Richter, Validation, verification, and benchmarking of crystal growth simulations, Journal of Crystal Growth 474 (2017) 171-177.

[2] K. Dadzis, O. Pätzold, G. Gerbeth, Model Experiments for Flow Phenomena in Crystal Growth, Crystal Research and Technology, 1900096 (2019).



Entwicklung von Kristallzüchtungsanlagen für die Validierung von multiphysikalischen Modellen.
Development of crystal growth setups for the validation of multiphysical models.

Die neue Definition des Kilogramms

In 2019 ist das neue Internationale Einheitensystem (SI) in Kraft getreten. Neben Ampere, Kelvin, Mol und Co. wird ab sofort nun auch das Kilogramm über eine Naturkonstante definiert. Damit hat auch das seit 130 Jahren als Maß aller Dinge geltende Ur-Kilogramm in Paris ausgedient. Eine besondere Rolle kam dabei den am Leibniz-Institut für Kristallzüchtung (IKZ) gezüchteten Einkristallen aus dem hoch angereicherten Isotop Silizium-28 zu.

Bereits am 16. November 2018 wurde auf der 26. Generalkonferenz für Maße und Gewichte in Paris das neue Internationale Einheitensystem (SI) beschlossen. Nun trat das System am 20. Mai 2019, dem Weltmetrologietag, offiziell in Kraft. Von jetzt an bilden 7 Naturkonstanten das Fundament allen Messens.

Das Kilogramm wird nun über die Planck-Konstante bestimmt, davon profitieren vor allem die Wissenschafts- und Hochtechnologie-Communities. Das IKZ hatte einen entscheidenden Anteil daran, dass der fast 130 Jahre alte Prototyp des Ur-Kilogramms abgelöst wird, denn die am IKZ gezüchteten hochperfekten Kristalle aus nahezu isotopenreinem Silizium-28 (^{28}Si, Anreicherung bis zu 99,9995 %) waren für die Neudefinition von entscheidender Bedeutung.

Bei diesen Kristallen haben nahezu alle Atome die gleiche Masse und sind in einem regelmäßigen dreidimensionalen Gitter angeordnet, was eine sehr genaue Zuordnung zwischen der Masse des Kristalls und der Zahl seiner Atome ermöglicht. Aus diesem Zusammenhang konnte der Wert der Avogadro-Konstante, die die Teilchenzahl pro Stoffmenge (Mol) angibt, mit nie dagewesener Präzision abgeleitet werden. Im neuen SI wird der Wert der Avogadro-Konstante festgelegt und ein Mol enthält deswegen genau $6{,}02214076 \times 10^{23}$ Einzelteilchen. Über die Avogadro-Konstante lässt sich dann auch der Wert der Planck-Konstante bestimmen – und entsprechend die Definition des Kilogramms bestätigen.

Insgesamt werden nun alle sieben Basiseinheiten über Naturkonstanten definiert. Bei der Sekunde (mit dem Hyperfeinstrukturübergang des Grundzustands im Cs-Atom), beim Meter (über die Lichtgeschwindigkeit) und bei der Candela (über das photometrische Strahlungsäquivalent einer speziellen Strahlung) ist dies bereits seit vielen Jahrzehnten der Fall. Nun ziehen auch die übrigen Einheiten nach, wobei hier die Elementarladung (für das Ampere), die Boltzmann-Konstante (für das Kelvin), die Avogadro-Konstante (für das Mol) und die Planck-Konstante (für das Kilogramm) die entscheidenden Rollen spielen.

Im Kontext des KILOGRAMM-Projekts in einer Floating Zone Anlage gezüchteter Prototyp eines Silizium-28 Einkristalls (Quelle: IKZ)

Im Rahmen der von der Physikalisch-Technischen Bundesanstalt in Braunschweig (PTB) geführten „KILOGRAMM"-Projekte wurden aus den im IKZ nach dem Float-Zone-Verfahren (FZ) gezüchteten ^{28}Si-Kristallen mehrere sehr präzise Kugeln mit weniger als 20 nm Formabweichungen bei rund 94 mm Durchmesser und mit einer defektfrei polierten Oberfläche präpariert. Unter diesen Voraussetzungen gelang es der PTB, die Zahl der ^{28}Si-Atome, die eine Kristallkugel von 1 kg Gesamtmasse ergeben mit der geforderten Unsicherheit von weniger als 2×10^{-8} zu bestimmen.
Sie beträgt: $2{,}152538397 \times 10^{25}$ Atome Silizium-28

Um die notwendige Reinheit der aus diesem Material gezüchteten Kristalle zu gewährleisten, sind diverse materialintensive Schmelzzonen-Reinigungsschritte notwendig. Die besonderen Herausforderungen waren deshalb der ca. 1000-fach höhere Materialpreis gegenüber herkömmlichem Silizium sowie die begrenzte Stoffmenge.

Silizium gilt als ein sehr umfassend untersuchtes Halbleitermaterial, das weltweit die Mikroelektronik und damit die Kommunikationstechnologien dominiert. Das IKZ wird weiterhin an den extremen Anforderungen für die weitere Verbesserung der Materialeigenschaften arbeiten, um künftige Anwendungen wie künstliche Intelligenz und Quantentechnologien zu ermöglichen. *„Die im Rahmen dieses Metrologie-Projektes entwickelte Expertise des IKZ zu isotopenreinen Si Kristallen erlaubt uns, künftig eine zentrale Rolle als Materialforschungsinstitut bei der Entwicklung innovativer Quantentechnologien einzunehmen"*, so Prof. Dr. Thomas Schröder, Wissenschaftlicher Direktor des IKZ.

The kilogram redefined

In 2019, the new International System of Units (SI) became operational. In addition to Ampere, Kelvin Mol and Co., the kilogram also is now defined by a natural constant. With this, also the international kilogram prototype which has been the standard for 130 years, has now become obsolete. A key role in this process was played by single crystals grown from the highly enriched isotopic silicon-28 at the Leibniz-Institut für Kristallzüchtung.

The new International System of Units (SI) had already been adopted at the 26th General Conference on Weights and Measures on 16 November 2018, and came into force on the World Metrology Day, 20 May 2019. From now on, seven natural constants establish the foundation of all measures.

For the kilogram, the new definition is based on the Planck constant. This is mostly beneficial for the scientific and high-tech communities. The IKZ played an important role in replacing the original kilogram prototype, since the structurally perfect crystals of nearly isotopically-pure silicon-28 (^{28}Si, enrichment up to 99.9995 %) grown at the IKZ were essential for the redefinition.

In these crystals, nearly all atoms have the same mass and are arranged in a regular three-dimensional lattice, which allows a very precise correlation between the mass of the crystal and the number of its atoms.

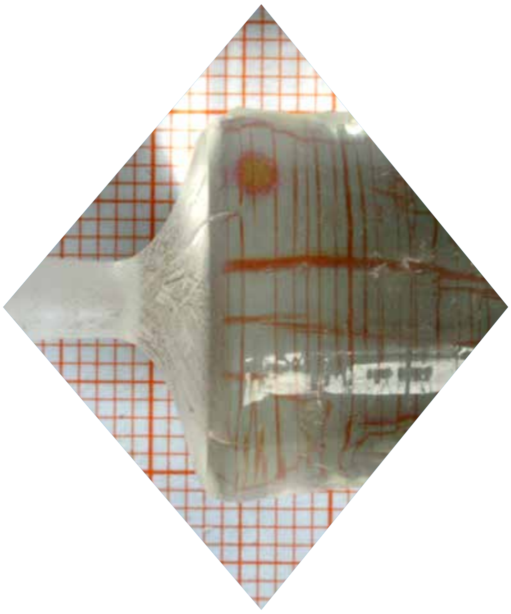
From this relation, the value of the Avogadro constant – which gives the number of atoms in a certain amount of substance (the mole) – could be derived with unprecedent precision. In the new SI system, the value of the Avogadro constant is now determined such that one mole contains exactly 6.0214076×10^{23} individual particles. From this it was possible to determine the Planck constant more precisely, confirming the new definition of the kilogram.

Now all seven basic units are defined by natural constants. This has been the case for many years for the second (with the hyperfine structure transition of the ground state in the Cs atom), the metre (via the speed of light) and the candela (via the photometric radiation equivalent of a special radiation). Now the other units also follow, whereby here the elementary charge (for the ampere), the Boltzmann constant (for the Kelvin), the Avogadro constant (for the mole) and the Planck constant (for the kilogram) play the decisive roles.

Within the framework of the "KILOGRAM" projects led by the Physikalisch-Technische Bundesanstalt (PTB) in Braunschweig, several very precise spheres with shape deviations of less than 20 nm at a diameter of about 94 mm and with a defect-free polished surface were prepared from the ^{28}Si crystals grown at IKZ using the float-zone method (FZ). Under these preconditions, PTB succeeded in determining the number of ^{28}Si atoms in a crystal sphere of 1 kilogram total mass, with the required uncertainty of less than 2×10^{-8}
It amounts to: $2.152538397 \times 10^{25}$ atoms of silicon-28

In order to guarantee the required purity of the crystals grown from this material, various material-intensive molten-zone cleaning steps had been necessary. The special challenges were therefore the approximately 1000 times higher material price compared to conventional silicon as well as the limited amount of material available.

Silicon is regarded as a very comprehensively investigated semiconductor material that dominates microelectronics and thus communication technologies worldwide. The IKZ will continue to work on the extreme requirements for the further improvement of material properties in order to enable future applications such as artificial intelligence and quantum technologies. *"IKZ´s expertise on isotope pure Si crystals, developed during this metrology project, will allow us to play in the next round a key role as materials science institute for the development of innovative quantum technologies"*, states Prof. Dr. Thomas Schröder, Scientific Director at IKZ.



Volume Crystals

Volume Crystals

Bulk crystal growth of KTb_3F_{10} for laser applications

D. Schulz, D. Klimm, K. Helm-Knapp, and M. Bickermann

Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Faraday isolators are among the key components for high-power lasers with emission in the near infrared (NIR), e.g. in materials processing. However, the performance parameters of the current ultra-short pulse disk lasers already reach the application limits of the current isolator material TGG ($Tb_3Ga_5O_{12}$). The required further power scaling can only be achieved by new materials that have lower absorption and show less thermal lensing compared to TGG. KTF (KTb_3F_{10}) crystals were presented in 2016 by Northrop Grumman Synoptics (USA) as superior high-performance isolators [1,2]. KTF has a cubic structure, just as TGG. First samples are being sold, but KTF cannot yet be manufactured reproducibly in the required quality.

The IKZ is investigating the growth of KTF single crystals as part of the BMBF-funded photonics project "IsoNova". We started research in 2017 and produced the first crystals that meet the specifications in 2019. However, crystals must be grown from non-stoichiometric melts and reports on proper growth conditions are lacking. We found that the chemically transient process conditions during the growth must be optimized within a narrow process window. Scattering and absorption centers in the crystal must be reliably minimized to develop marketable prototype material [3]. But until their origins and chemical nature are fully understood, the challenges to purity and process control remain a moving target.

KTF crystals are grown by the Czochralski technique with inductive heating; the melt is contained in platinum or in graphite crucibles. In literature, just a few reports on the phase diagram for KF-TbF_3 are found, with quite inconsistent data. Based on thermochemical analysis, we could however derive that crystal growth requires an excess of approximately 2 mol% KF in the melt (what is then actually a solution). During the crystal growth, KF accumulates in the remaining liquid. This influences the quality of the growing crystal, as the formation and incorporation of neighboring, KF-rich phases increase with the crystal length. When they form scattering centers, this results in a deterioration of the optical properties. KF accumulation is also impacts the maximum yield, i.e. crystallizable fraction of the melt.

Another issue is contamination with oxygen. The starting materials potassium fluoride (KF) and terbium fluoride (TbF_3) are known to easily react with moisture resulting in formation of unwanted oxygen-containing phases that can act again as scattering or absorption centers. We found out that commercially available powder material is not appropriate for high-quality KTF crystal growth. We have developed a process to provide highest purity state-of-the-art material using our dedicated fluorination station where the powders are subjected to a hot flow of gaseous hydrogen fluoride (HF) and subsequently compacted to a bulk that is less affected by moisture in air during the transfer to the growth station.

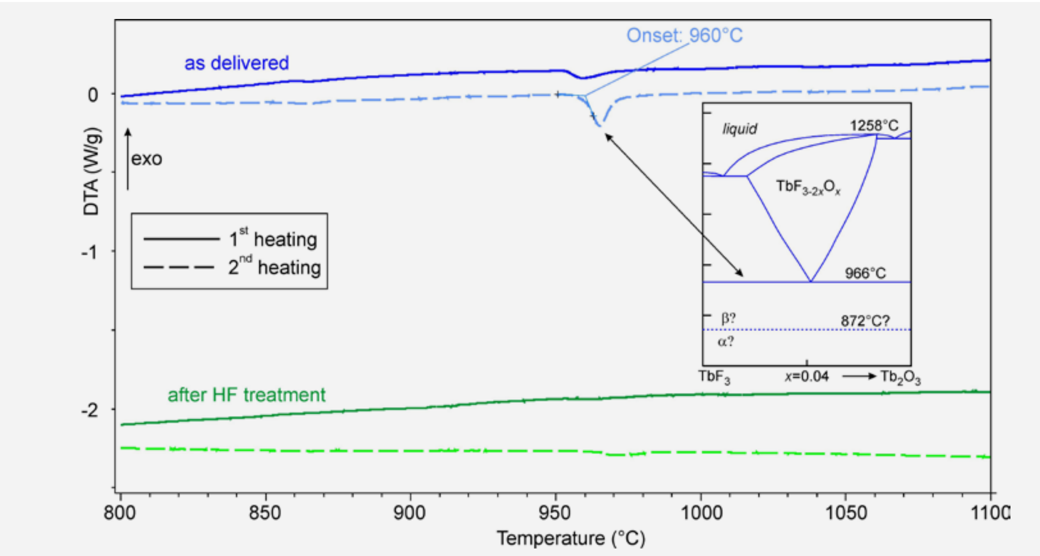


Fig. 1
Differential thermal analysis (DTA) of a commercial TbF_3 powder charge before (blue) and after (green) fluorination; two heating cycles are shown, respectively; the inset shows a part of the phase diagram TbF_3-Tb_2O_3 with an oxyfluoride phase that melts at around 966°C.

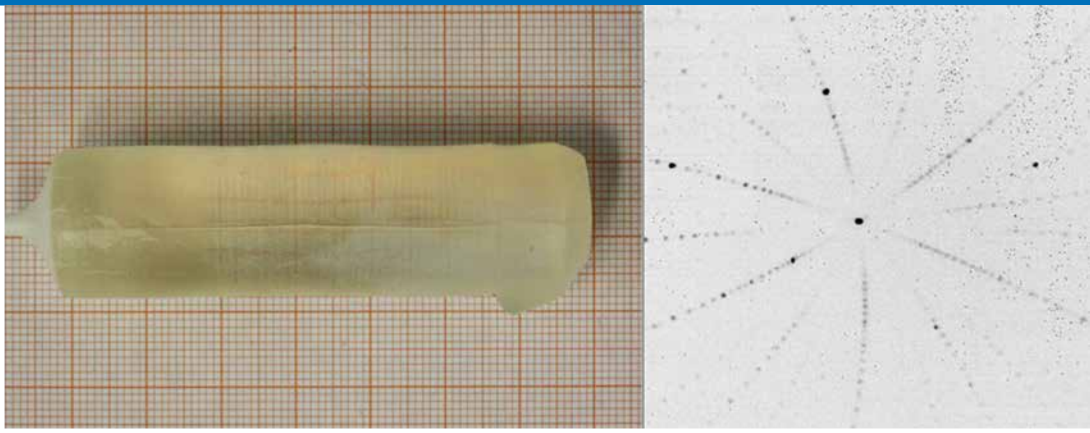


Fig. 2
KTF single crystal grown in <111> direction (20 mm diameter, 70 mm length, growth direction is left to right) and corresponding Laue X-ray back-scattering diffraction pattern (provided by A. Kwasniewski)

But fluorination is a slow batch process, and several runs are required to prepare the starting material for just a single growth run. That is why we will upgrade our fluorination capabilities in 2020. Finally, Fig. 1 shows the limits of this process: While fluorination effectively removes the terbium oxyfluoride melting peak appearing at 960°C, repeated heating under high-purity inert gas leads to traces of re-oxidation of the TbF_3. Crystal growth must take place under very dry conditions in a high-vacuum tight growth station.

A third issue is evaporation from the melt surface. It makes the crystal surface appear frosted, but that is not the primary concern. We observe a preferred evaporation of KF that influences the actual composition of the melt. To minimize the loss of KF from the melt, a special geometry is employed in the growth setup that ensures low overheating at the melt surface. However, the usable length of the crystal shown in Fig. 3 is restricted to ca. 40 mm, as in the lower part of the crystal, the incorporation of second phases is leading to a decrease in optical transmission. The transient of chemical composition during growth is still under investigation. In contrast, Fig. 3 shows an as-grown KTF single crystal with high optical transparency and clear surface. Measurements have shown that in this crystal the density of scattering centers is even lower than in commercial isolator material.

Different optical techniques are used to assess the optical transmission and other parameters that are decisive for the NIR isolator application. Apart from scattering centers, also the residual absorption must be as low as possible to prevent internal heating under laser irradiation. We are currently investigating the origin of residual absorption in the NIR range and the impact of other rare-earth elements that might be trace impurities in the crystals. In summary, crystal growth of KTF comprises a lot of challenges. We were able to demonstrate a first crystal that exceeds the commercial standard. However, preparation of reliable prototype material requires intensive further research and improvements in growth technology as well as in identification of scattering and absorption centers.

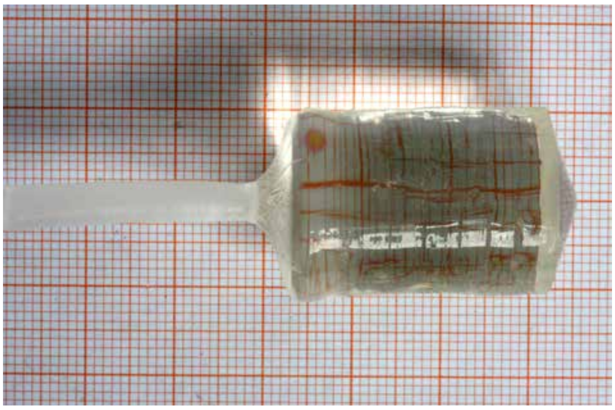


Fig. 3
Single crystal of KTF grown by the Czochralski technique (20 mm diameter, 25 mm length, growth direction is left to right)

References

[1] K.T. Stevens W. Schlichting, G. Foundos, A. Payne and E. Rogers, *Promising Materials for High Power Laser Isolators,* Laser Technik Journal 3/2016, pp. 18-21

[2] W. Schlichting, K. Stevens, G. Foundos, A. Payne, *Commercializing potassium terbium fluoride, KTF (KTb_3F_{10}) faraday crystals for high laser power optical isolator applications*, Proc. SPIE 10448 [Optifab 2017] 104481N

[3] A.A. Jalali, E. Rogers, K. Stevens, C*haracterization and extinction measurement of potassium terbium fluoride single crystal for high laser power applications*, Optics Letters 42 [5] (2017) 899-902

New large-lattice-parameter perovskite single-crystal substrates

C. Guguschev[1], D. G. Schlom[2,3], M. Brützam[1], D. Klimm[1], H. Paik[2,4], S. Ganschow[1], and M. Bickermann[1]

[1] Leibniz-Institut für Kristallzüchtung, Berlin, Germany
[2] Department of Materials Science and Engineering, Cornell University, Ithaca, USA
[3] Kavli Institute at Cornell for Nanoscale Science, Ithaca, USA
[4] Platform for the Accelerated Realization, Analysis, & Discovery of Interface Materials (PARADIM), Cornell University, Ithaca, USA

Functional oxide thin films are of strong contemporary interest in materials physics. Examples include La-doped $BaSnO_3$, a semiconducting oxide exhibiting a very high electron mobility, $LaInO_3$ as a gate oxide because of its high dielectric constant, $BiScO_3$ as an important constituent of a new class of high-temperature piezoelectrics and $PbZrO_3$ as an antiferroelectric material relevant to energy storage. These materials all possess a perovskite crystal structure with (pseudo-)cubic lattice parameters in slight excess of 4.1 Å, for which no large-area substrate crystal had been available yet. As a result, current studies are mostly based on highly lattice-mismatched substrates leading to films with low structural quality, which in turn drastically degrades their electronic performance in proof-of-principle devices.

This situation is about to change, as the IKZ and the Cornell University worked together to invent a novel bulk crystal growth technique tailored to the new double-perovskite Ba_2ScNbO_6 with cubic structure (space group $Pm\bar{3}m$) and a lattice parameter of 4.11672(1) Å [1]. Such development was of vital importance due to the appearance of very intense growth instabilities during Czochralski growth, most probably caused by reduction of the niobium oxidation state in the crystal with consequential darkening, absorption and impeded radiative heat transfer from the interface passing through the crystal. The new approach is based on a rf-heated iridium crucible embedded in ZrO_2 and Al_2O_3 insulation and one of the key elements which made it possible is the additional thermal insulation, e.g. in shape of a disc, added to the central region above the surface of the melt. It reduces the heat loss below and ensures the nucleation of Ba_2ScNbO_6 crystals at the coldest spot near or at the crucible wall. The grain-selection and continuous grain enlargement towards the central part of the crucible during cooling of the growth setup is maintained by a suitable temperature distribution in the melt held inside the crucible.

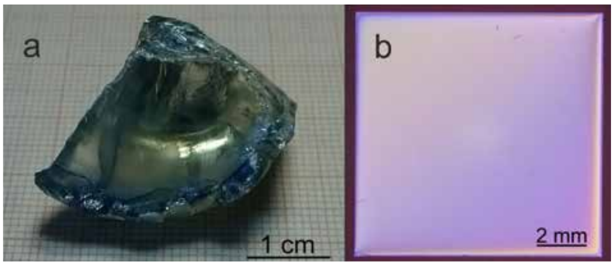


Fig. 1
a) Ba_2ScNbO_6 single crystal containing multicrystalline regions at the rim [1].
b) DIC micrograph of a chemo-mechanically polished (1 0 0)-oriented single-crystal wafer of Ba_2ScNbO_6 with a surface area of 10×10mm² prepared from the crystal shown in (a). The dark lines are caused by dust particles sitting on the surface. The substrates were oriented, cut, and polished by CrysTec GmbH, Berlin.

The growth conditions are suitable to yield relatively large crystals (see Fig. 1a) and (100)-oriented single-crystalline substrates with surface areas as large as 10x10 mm². Fig. 1b shows a differential interference contrast (DIC) micrograph of a representative substrate. With measured rocking curve FWHM values in the 21-33 arc sec range, the Ba_2ScNbO_6 substrates are of high structural quality.

While the composition was chosen on a lattice parameter survey, the ability to grow the crystal from the melt was assessed by a thermo-chemical study. The analysis showed that Ba_2ScNbO_6 melts at a relatively high temperature of about 2165 °C and in an inert atmosphere it is accompanied by a significant mass loss of 1 %. The corresponding differential thermal analysis (DTA) and thermogravimetric (TG) curves are shown in Fig. 2. The material loss is mainly caused by evaporation of BaO, since this component has by far the highest vapor pressure (20 mbar) of all involved evaporating species. Although a significant depletion of Ba and oxygen takes place, it was no detrimental factor regarding our single crystal growth technique on a larger scale. The achievement was published recently [1] and a joint patent has been applied for (US reference number: 16/424,987).

Volume Crystals

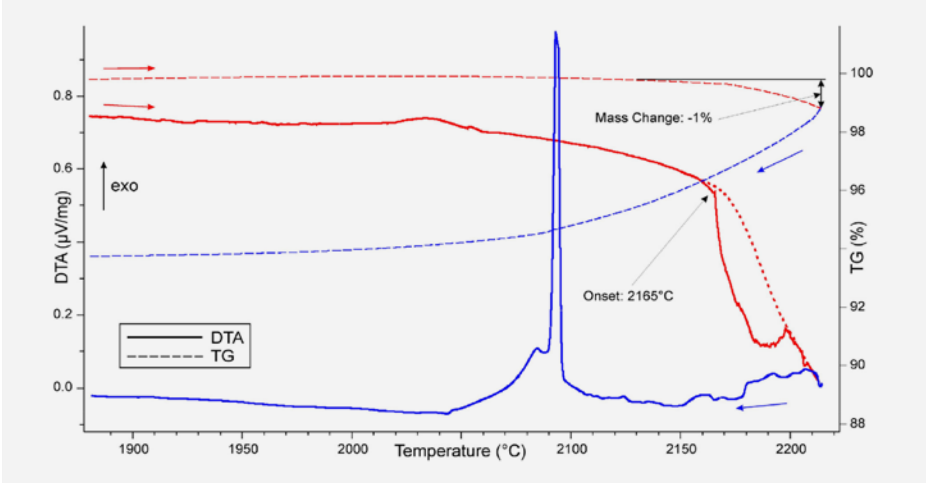


Fig. 2
Measured DTA and TG curves of a Ba_2ScNbO_6 sample in the temperature range of ca. 1880 – 2210 °C during heating (red curves) and cooling (blue curves). The strong exothermal peak indicates crystallization near 2095 °C, which means ca. 70 K supercooling below the melting point [1].

The second achievement is based on a crystal growth development in a complex quaternary material system. We demonstrated recently, that $(La,Nd)(Lu,Sc)O_3$ single crystals can be grown from the melt at temperatures of about 2170°C by using the Czochralski technique [2]. The new solid-solution crystal offers a pseudocubic lattice parameter of about 4.09 Å and due to its flexibility in the lattice, the accessible lattice parameter range is relatively broad. So far, this material offers the largest available volumes (Fig. 3) to fabricate large-lattice-parameter substrates with dimensions 10 mm × 10 mm very close to the desired lattice parameter range. We achieved single crystals with diameters up to 17 mm and total lengths up to 50 mm. Despite the very complex composition, a good chemical homogeneity was achieved. Compared to the Ba_2ScNbO_6 crystals, the structural quality is slightly lower, since the crystals are not yet free of subgrains.

Initial films grown by MBE on the new Ba_2ScNbO_6 and $(La,Nd)(Lu,Sc)O_3$ single-crystal substrates at Cornell University have already demonstrated the strong impact and benefit of using lattice-matched high-quality substrates. For example, the first epitaxial La-doped $BaScO_3$ films grown directly on the chemo-mechanically polished surfaces (without applying any substrate termination recipes) exhibited mobilities of 192 and of 181 $cm^2V^{-1}s^{-1}$ [2,3] respectively. The level of mobility reached is higher than in any report in the literature and is indicative of the electron mobility that can be achieved in electronic devices utilizing these films, e.g., a field-effect transistor.

Acknowledgements

The authors would like to thank T. M. Gesing, M. Gogolin, V. J. Fratello, T. Markurt, A. Kwasniewski, D. J. Kok, A. Dittmar, U. Jendritzki, Z. Chen and D.A. Muller for their kind support and fruitful collaboration.

References

[1] C. Guguschev, D. Klimm, M. Brützam, T.M. Gesing, M. Gogolin, H. Paik, A. Dittmar, V.J. Fratello, D.G. Schlom, *Single crystal growth and characterization of Ba_2ScNbO_6 – A novel substrate for $BaSnO_3$ films,* Journal of Crystal Growth, 528 (2019) 125263.

[2] C. Guguschev, D. Klimm, M. Brützam, T.M. Gesing, M. Gogolin, H. Paik, T. Markurt, D.J. Kok, A. Kwasniewski, U. Jendritzki, D.G. Schlom, *Czochralski growth and characterization of perovskite-type $(La,Nd)(Lu,Sc)O_3$ single crystals with a pseudocubic lattice parameter of about 4.09 Å,* Journal of Crystal Growth, 536 (2020) 125526.

[3] H. Paik et al., *High mobility La-doped $BaSnO_3$ thin film growth on lattice-matched $Ba(Sc_{0.5},Nb_{0.5})O_3$ (001) substrate by molecular-beam epitaxy,* poster at the 19th International Conference on Crystal Growth and Epitaxy (ICCGE-19/OMVPE-19), July 28 – August 2, 2019, Keystone, Colorado, USA.

Fig. 3
$(La,Nd)(Lu,Sc)O_3$ single crystal grown by the Czochralski technique [2].

Growth of single crystals by the silicon granulate crucible method

R. Menzel, K. Dadzis, A. Nikiforova, L. Lehmann, M. Renner, U. Jendritzki, N. Lorenz-Meyer, B. Faraji-Tajrishi, U. Juda, K. Irmscher, N. Abrosimov, and H. Riemann

Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Fig. 1

Silicon single crystals with ultrahigh purity and crystalline perfection are crucial for applications in power electronics or photovoltaics. In 2019 the FZ-Si group at IKZ has successfully completed the three-year research project "SiGrEt" (**Si**lizium **Gr**anulat **E**igen**t**iegelverfahren), which was funded by the Leibniz Association in frame of the Leibniz Wettbewerb. The aim of the project was to demonstrate the growth of large silicon volume crystals with a high purity at the level of Float Zone (FZ) silicon, using a new growth concept – the **Si**licon **Gr**anulate **C**rucible (SiGC) method. The SiGC growth concept combines the advantages of the industrial established methods for the production of silicon single crystals, namely the FZ method (ultra-high purity and homogenous axial dopant distribution achievable in an energy-efficient growth process) and the Czochralski method (lower feedstock cost and less diameter limitations compared to FZ). Fig. 1 shows a SiGC crystal with 4 inch diameter. As in FZ, the developed setup allows stable growth without contamination.

The SiGC method shares many similarities with FZ and is derived from the crucible-free pedestal growth principle. In contrast to these methods, for the SIGC process no expensive Siemens feed rods are needed, which also limit the crystal diameter. The process is continuously replenished with silicon granules, which can be produced at low cost in the fluidized bed reactor (FBR).

During SiGC growth the melt is heated using high-frequency (f=2MHz) inductive heating and is not in contact to contaminating crucible, but rests in a silicon "self-crucible" that stabilizes in a bed of FBR granules. A main task in the project was to find suitable growth parameters for the applied starting procedure shown in Fig.2.

A major challenge in this context was to overcome the following three process destabilizing impact factors:
1. Insufficient melting of silicon granules replenished to the melt pool leads do generation of defects and grain boundaries when unmolten particles get in contact with the triple-phase line. Counter-measures as high heating power and lower spindle rotation rate that drive a melt flow away from the three-phase line, allow to avoid this event.
2. Fluctuations of the melt filling level cause crystal diameter instabilities. For stable growth conditions, the melt filling level must be kept constant within a range of only a few millimeters. A rise or fall of the melt filling level results from improper replenishment rates or abrupt changes of the self-crucible volume, when melt is flowing into voids in lower regions of the granulate bed. The self-crucible shape can be stabilized by forming a thick solid silicon layer between melt and granular bed during generation of the melt pool.
3. Melt vibrations with a frequency of about 1 Hz may lead to loss of single-crystalline structure, especially during the Dash-necking process when the free melt surface area is very large. The negative effect of melt vibrations is known from FZ growth. Its origin is not certainly known but probably related to the electromagnetic forces generated in the melt.

For the industrial production a high process stability and reproducibility is needed to ensure an economic rate of yield. In frame of a master thesis by N. Lorenz-Meyer, a model-based control system for the process was developed [1]. The model is analytically deduced based on the hydromechanical, geometrical and thermal conditions of the process. Experiments were conducted to identify unknown model parameters and to validate the model. We were able to verify the physical consistency of the model using simulation studies with a prediction error below 2%.

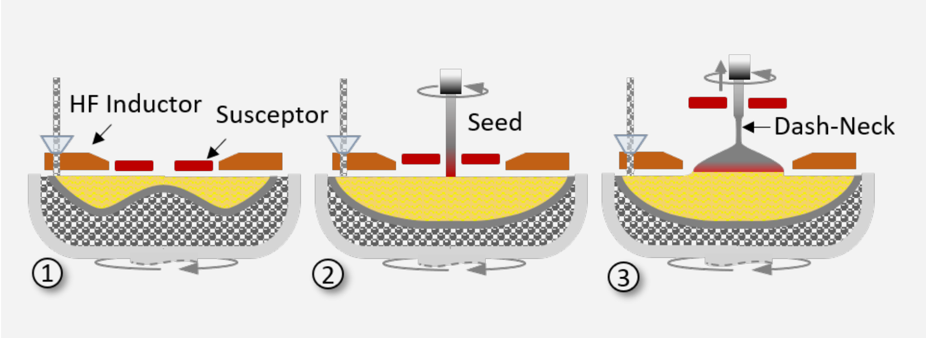


Fig. 2
SiGC starting procedure:
1. Generation of melt pool using inductive heating and susceptor,
2. Seeding with Dash-necking process
3. Growth of crystal cone and cylindrical growth phase.

SIGC crystals have been characterized with respect to defect contents and material purity [2]. A low oxygen concentration < 10^{16} atoms/cm³ was measured using FTIR. This value is comparable to FZ crystals and shows that oxygen evaporates from the free melt surface during SiGC growth. With a concentration of about 10^{17} atoms/cm³, the carbon concentration measured using FTIR was significantly higher than what is achievable in the standard FZ process. There is strong evidence that the increased carbon levels stem from the granulate raw material, which has higher carbon content compared to the Siemens feed rods used for FZ. Silicon granulate particles used as feedstock can be described as microscopically porous nanocrystalline material. This structure increases the electrical resistivity of granulate to the level of intrinsic silicon even at low temperatures (reaching $3 \cdot 10^5$ Ωcm), which is relevant for inductive melting of granulate. The dopants in granulate are partly compensated and lead to a resistivity of about 150 Ωcm in crystalline samples. Gas doping with PH_3 during crystal growth allows to achieve homogeneous resistivity distributions, but an adjustment of the dopant inflow as well as further analysis of the melt flow on the radial distribution are necessary. As shown in Fig. 3, impurity analysis of granulate feedstock using ICP-MS revealed relatively high concentrations of transition metals with the sum of 14 analyzed elements reaching $2 \cdot 10^{15}$ cm-³. In the grown crystals this value decreased approximately by one order of magnitude leading to an average effective segregation coefficient of 0.1. This value is much higher than the equilibrium coefficients in the range 10^{-4}–10^{-6} and may be caused by the interaction between metals and extended defects or other currently unclear reasons.

A Si-GC crystal was used as a feed rod in an FZ growth process to obtain a dislocation-free crystal where the metals have been segregated once again. ICP-MS measurements indicated a decrease of the total concentration of transition metals from $3 \cdot 10^{13}$ - $3 \cdot 10^{14}$ cm³ in Si-GC crystals to $2 \cdot 10^{13}$ cm^{-3} in the FZ crystal. Carrier lifetime measurements showed a level of 300 µs, which increases to a very high value of almost 20 ms after the surface passivation.

It can be concluded that the SiGC process allowed growth without contamination. Increased impurity levels of oxygen and carbon are related to the raw material impurity content. The SiGC process will be further developed for the use of low-cost raw material with higher purity and different form factor.

References

[1] N. Lorenz-Meyer, R. Menzel, K. Dadzis, A. Nikiforova, H. Riemann; *Lumped parameter model for silicon crystal growth from granulate crucible,* Crystal Research & Technology (accepted)

[2] K. Dadzis, R. Menzel, U. Juda, K. Irmscher, C. Kranert, M. Müller, M. Ehrl, R. Weingärtner, C. Reimann, N. Abrosimov, H. Riemann; *Characterization of silicon crystals grown from melt in a granulate crucible*, Journal of Electronic Materials (accepted)

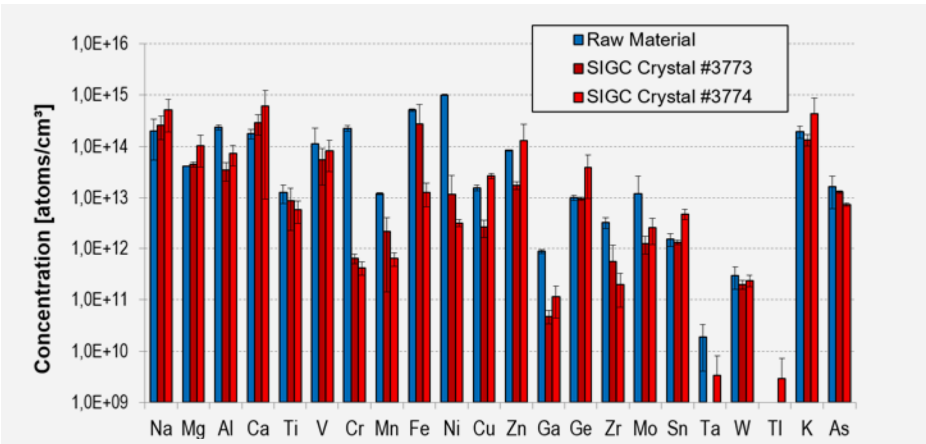


Fig. 3
Results of High Resolution Inductively Coupled Plasma - Mass Spectrometry (HR-ICP-MS)

Volume Crystals

High-yield reduction process of natural and enriched GeO_2: en-routing for HPGe crystals

K.-P. Gradwohl, A. Gybin, J. Janicskó-Csáthy, J. Klose, and R. Radhakrishnan Sumathi

Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Fig. 1a
Reduction equipment in operation for reducing and converting powders into metal bars

High purity germanium (HPGe) with ultra-low impurity in parts per trillion level is of demand for radiation detectors, applications in *x*-ray, g-ray physics, astronomy, etc. IKZ is a member of international LEGEND [1] collaboration, which aims to resolve the question whether neutrinos are their own antiparticles and thus significantly expedite our current understanding of the structure of matter and the development of the universe. Detectors fabricated from natural or enriched ^{76}Ge crystals with ultra-high purity are vital to observe this extremely rare decay process – the neutrinoless-ßß-decay. Among the five isotopes of Ge, the abundance of ^{76}Ge in natural Ge is merely 7%. However, this isotope is having a radioactivity decay with a half-life period of over 10^{21} years. To detect such a rare occurrence, very high purity Ge detectors with extremely low background are necessary.

In the extraction steps of Ge, germanium di-oxide (GeO_2) is the intermediate product. Subsequently, GeO_2 has to be reduced by hydrogen (H_2) to obtain Ge metal. There are only limited optimized processes accessible/available for reduction with reasonable yield and one needs especially a very high-yield process for isotopic ^{76}Ge due to the extremely high material-cost.

In addition, the main challenge in the reduction of $^{76}GeO_2$ is to minimise the cosmogenic exposure to the material. Any exposure of cosmic rays has to be absolutely curtailed at any given processing step, since it gives raise to ^{68}Ge and ^{60}Co isotopes that generate an internal contamination in the ^{76}Ge material, which in turn increases the background noise in the region of interest of the spectrum in the detectors. This requisite, together with high material cost requires a development of processes that is both rapid and material-efficient.

At IKZ a new reduction equipment (Fig.1a) has been commissioned, which can be operated at high temperatures under H_2 atmosphere. The in-house reduction of GeO_2 allows better control over the impurities in the Ge source material. In addition, it will bring-in a full value proposition under one roof, covering the process steps from GeO_2 powder reduction up to providing high purity (13N) crystals (i.e. in the form as detector-blocks). This closed furnace is controlled by programmable logic controller (PLC) and has a fused silica (quartz) tube. This quartz tube is extremely resistant to thermal shocks compared to alumina tubes. Hence one can operate rapidly the heating and cooling procedures.

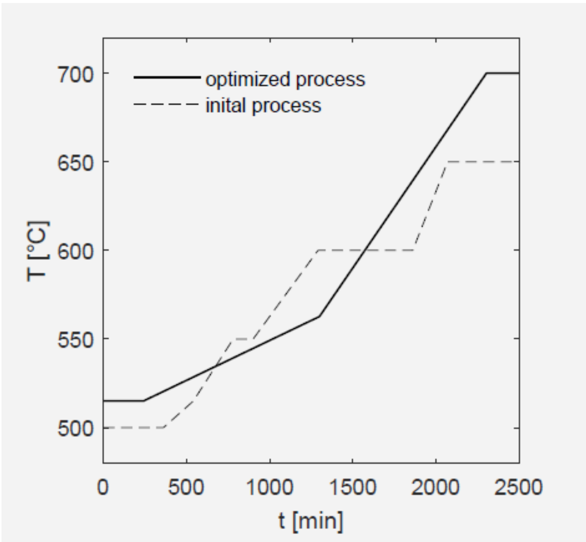


Fig. 1b
Temperature profile of the reduction processes: initial process (dotted-line), optimized process (solid-line)

Volume Crystals

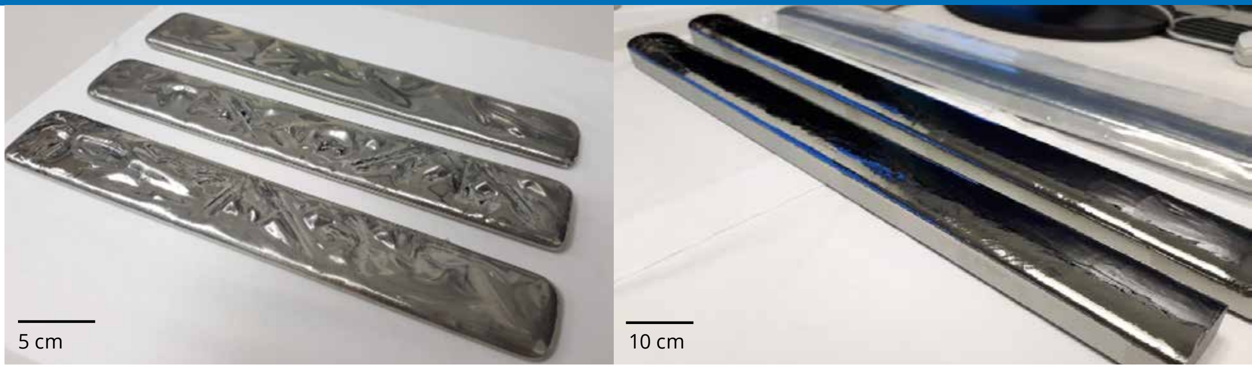


Fig. 2
(left) Reduced Ge (4N) metallic bars; (right) reduced and then zone-refined Ge bars (intrinsic purity 6N)

A high-yield reduction process has been established by carrying out experiments under H_2 atmosphere with proper and strict safety measures. It may be noted that oxygen (O_2) induces explosion when mixes with H_2. To prevent possible air (O_2) getting into the equipment during operation, the experiments were carried out at slight overpressure than atmosphere (30 to 120 mbar more). Each experiment contains two process steps: (1) white GeO_2 powder is reduced into Ge powder, (2) subsequently, this grey Ge powder is melted to obtain Ge metallic bars. Graphite boats were used as containers to hold GeO_2 powder during reduction and melting. A mixture of H_2 and nitrogen (N_2) was used as a process gas with a flow rate of 200 l/h (for H_2) and 100 l/h (for N_2). In this reduction process, the reaction products are germanium and water vapor, GeO_2 + $2H_2$ à Ge + $2H_2O$. The reaction time depends on particle size of the powder. Average diameter of the particles is usually ~ 20 to 30 µm. We started the experiments initially with natural GeO_2 powder and investigated the process parameters. To obtain a shortened process time with high yield, we found an optimised process-temperature window with a constant, high reaction rate (500°C < T < 700°C) throughout the process (Fig.1b) and at the same time minimum evaporation of germanium monoxide (GeO). GeO will sublimate above 700°C and could deposit on the inner surface of the quartz tube (at the tube's rear end), which will greatly affect the yield. As a subsequent step, the melting procedure is initiated with quick heat ramp-up of 400°C/h to a temperature of 960°C, to melt the Ge powder and obtain Ge metal bars eventually (Fig. 2 (left)). The total process time starting from loading the oxide powder till to harvesting the Ge bars is 46 h. We were thus able to develop a successful single process with a very high yield of > 99% with typical capacity of 2 kg per process (i.e. 1 kg GeO_2 per boat).

Though the fine grey Ge powder in the reduction step is directly melted to Ge bars, it may still contain a high amount of chemical impurities. The obtained Ge bars usually show resistivities in the range of 1 - 10 W·cm as characterised by the four-point-probe method. The HPGe process requires at least an electronic grade (6N) Ge with > 47 W·cm resistivity as starting material.

So, the Ge bars obtained from reduction were purified by a home-built zone-refiner up to 6N purity. Ge has a favorable segregation coefficient (k) for most of the elements, therefore impurities move either to front or tail end of the zone refined bars (low resistivity tails) depending on their equilibrium (k_0) value. For each Ge-bar, multiple zone passes of up to 16 times were carried out with a zone-velocity of 5 mm/min. This resulted in a material with good resistivity (~50 W·cm) in the middle portion of the bars (Fig.2, right), corresponding to 70% yield out of the bars' total length. Very low resistivity portions are cut off for reuse and then again purified by repeated zone refining (ZR) (to reach a final yield (6N) of > 95%). These 6N bars will be the starting material for HPGe crystal growth.

After this successful establishment of the hydrogen reduction of natural GeO_2, the process was seamlessly transferred to reduce and zone refine ^{76}Ge material from the enriched (88%) oxide powder supplied by our co-operation partner, Technical University Munich (TUM). Twenty experiments were carried out to reduce 32.8 kg of $^{76}GeO_2$ to obtain 23 kg of ^{76}Ge. In this process development also, we were able to reach an average reduction yield of 99.85% [2]. The enriched ^{76}Ge bars with 6N purity have been handed over to TUM as part of IKZ's contribution to the LEGEND-200 collaboration experiment.

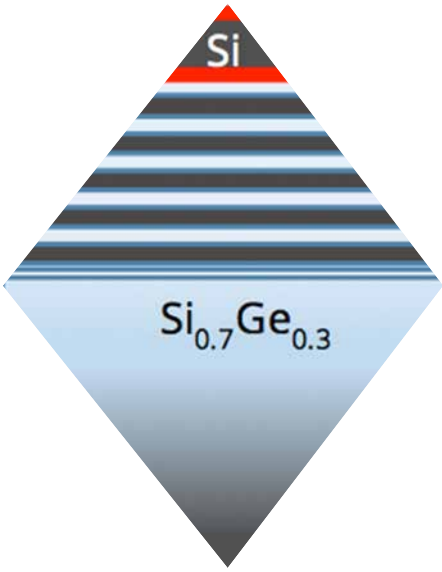
Acknowledgement

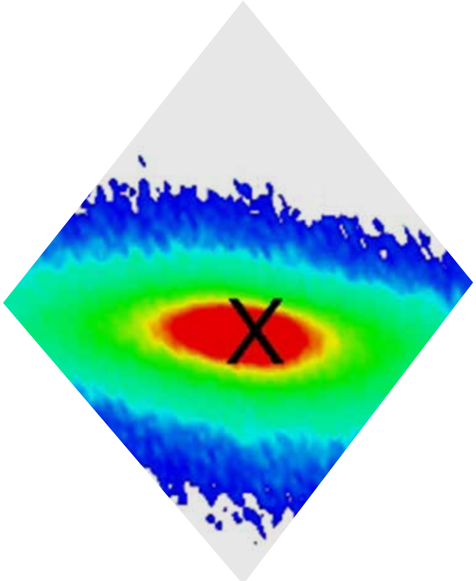
We thank the financial support provided by the German Federal Ministry for Education and Research (BMBF) for the financial support within the collaborative project under the grant number 05A2017-GERDA.

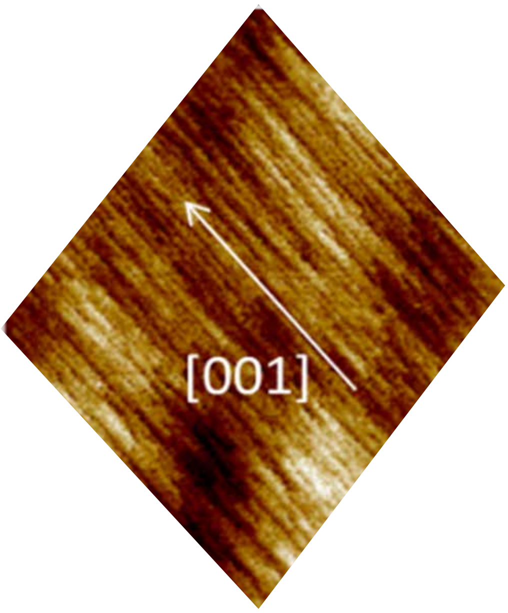
References

[1] http://legend-exp.org/

[2] K.-P. Gradwohl, J. Janicskó-Csáthy, O. Moras, S. Schönert, R. R. Sumathi, LEGEND collaboration meeting presentation, 2-6 Dec. 2019, Seattle, USA.







Nanostructures & Layers

Control of nucleation and growth of crystalline nanostructures

O. Ernst, F. Lange, D. Übel, T. Teubner, and T. Boeck

Leibniz-Institut für Kristallzüchtung, Berlin, Germany

The successful growth of nanostructures depends decisively on the control of the onset of crystallization on substrate surfaces, i.e. the investigation of wetting and nucleation phenomena. Here, the challenges range from the required area-wide growth of Si micro-crystallites to the locally ordered growth both of Cu(In;Ga)Se_2-microcrystallites and Ge nanowires. The distribution of crystallization points on the substrate surface has to be adapted to the intended purpose, i.e. randomly, but uniform in density, or specifically isometrically. In contrast, the heterogeneous nucleation has to be avoided for homogeneously strained monoisotopic ^{28}Si epitaxial layers of a few nanometers thickness.

Beyond the interest in basic research, potential applications are the motivation for these investigations.

Quantum computers are such a vision. The computational speed of IT infrastructure is crucial for the efficiency of complex data processing, as required for example in cryptography, modeling of new materials, sensor technology, communication, weather forecasting or logistics planning. Quantum computers are regarded as a key technology of the 21st century, using the superposition principle to allow for highly parallel computing and potentially solve problems quickly no conventional computer could solve in a feasible amount of time. Spin qubits in semiconductor materials as functional basic elements are promising candidates to realize such an approach due to the proven scalability. In this sense, we grow a thin strained Si layer between SiGe barriers by molecular beam epitaxy (MBE). Such a Si layer forms a quantum well for a two-dimensional electron gas. Top gates on such semiconductor structures finally form electrostatically the quantum dots, which are hosting single electrons for spin manipulation. Such operations at temperatures in the mK range are fragile. Beside external magnetic and electric noise the Si layer itself is a source of noise. Three major factors determine the quantum suitability of the Si layer: structural perfection, a low content of electrically active impurities (not more than 10^{14} cm^{-3}), and a low content of ^{29}Si isotopes.

Spin qubit dephasing is dominated by magnetic noise typically from the nuclear spin bath of ^{29}Si due to hyperfine contact interaction. The technology to grow highly enriched (>99.99%) and purified ^{28}Si bulk crystals developed by the IKZ for the former Avogadro project will be used here to get the necessary ^{28}Si evaporation sources for the MBE. The research is carried out within the frame of the Leibniz Competition project SiGeQuant in cooperation with the Leibniz-Institut für innovative Mikroelektronik (IHP), the Institute for Semiconductor Technology (IHT), and the JARA-FIT Institute for Quantum Information (IQI). Relations to many other national and international partners exist to realize qubit research in isotopically pure silicon 28.

Prerequisites for the implementation of the project are expertise in the handling of semiconductor nanostructures and a profound understanding of the physical and chemical processes during the growth of semiconductor nanostructures. The generation of silicon and germanium nanowires and the observation of their internal lattice strains [1] served as a model. These results will be used as a basis for the estimation of the desired stress in ^{28}Si layers required for project SiGeQuant (see Fig. 1) as well as for the studies already carried out on the influence of changes in surface energies and van der Waals interactions on other nanostructures. A corresponding publication has been submitted recently.

The investigation of wetting and nucleation processes plays a crucial role. Here, the theoretical approaches of local structure formation in systems far from equilibrium are to be put into practice. By considering the free energy, the stability or rather the instability of thin films can be predicted and exploited for the formation of layer or island structures. In the same way, the effective interface potential is considered to get a deeper insight into the mechanisms behind structure formation.

Nanostructures & Layers

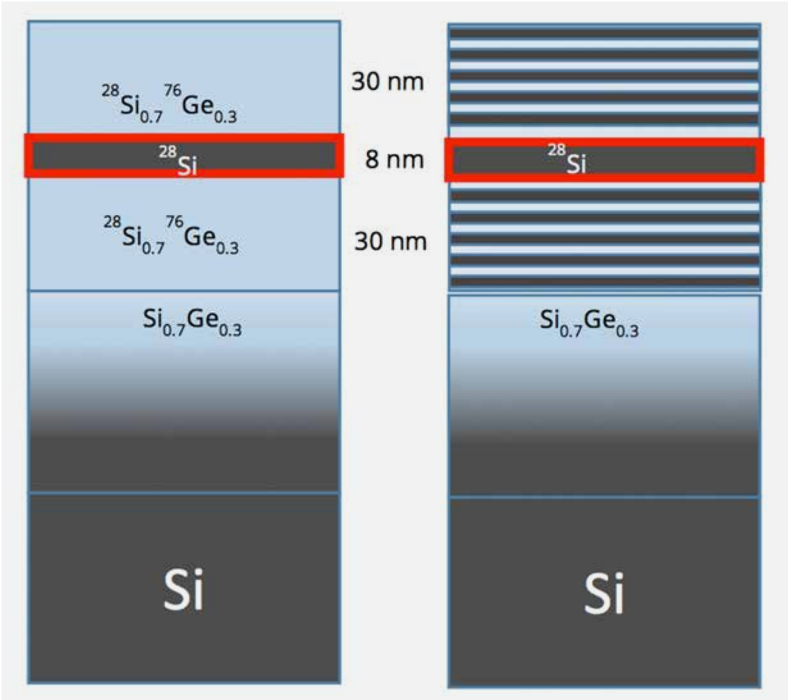


Fig. 1
Different approaches for
a) $^{28}Si_{0.7}{}^{76}Ge_{0.3}$ mixed layer, 8 nm = ^{28}Si (left);
b) $^{28}Si^{76}Ge$ superlattice (nominal 30 at% Ge) 30 nm = Ge_3Si_7 (right)

The localized structure formation for the realization of locally defined nano- and micro-semiconductor devices without the use of complex mask or lithography processes is an application. Focused laser radiation of suitable wavelength and intensity should lead to targeted thermal inhomogeneities in order to initiate selective nucleation on the locally heated surface. Semiconductor island structures created in this way can be used to achieve significant material savings in large-area modules for energy conversion. Both industrial partners and a number of research institutions are interested in the development of such structures. The project Kost-Sol is funded for the design and realization of a functional prototype of the experimental facility and is supported by the German Federal Ministry of Economics with a budget of 1.5 million €. The Federal Institute for Materials Research and Testing (BAM), the University of Duisburg/Essen are also partner of the project, as is Bestec GmbH, a company leading in construction of highly specialized UHV research equipment.

References

[1] F. Lange, O. Ernst, T. Teubner, C. Richter, M. Schmidbauer, O. Skibizki, T. Schröder, P. Schmidt, T. Boeck, *In-plane growth of germanium nanowires on nanostructured Si(001)/SiO_2 substrates,* Nano Futures, https://doi.org/10.1088/2399-1984/ab82a0

Nanostructures & Layers

Enhanced conductivity at the $LaInO_3/BaSnO_3$ interface

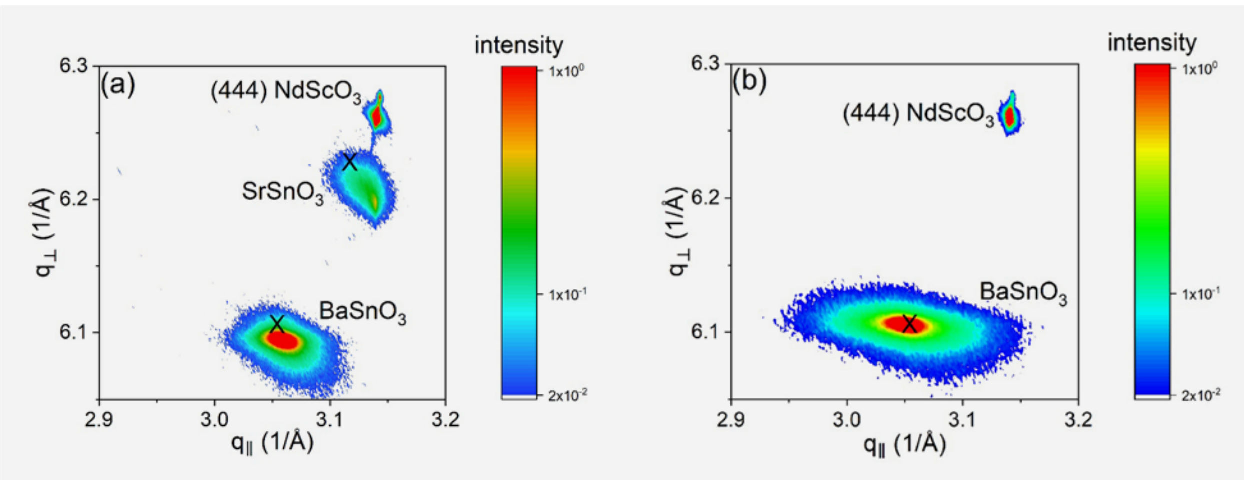
D. Pfützenreuter[1], R. Ravindran[1], S. Kim[2], A. Baki[1], K. Char[2], and J. Schwarzkopf[1]

[1] Leibniz-Institut für Kristallzüchtung, Berlin, Germany
[2] Department of Physics and Astronomy, Seoul National University, Seoul, South Korea

The development of novel concepts for faster non-volatile memories based on perovskite oxides has gained a lot of attention during the last years. A Ferroelectric field effect transistors (FeFET) based on a semiconductor channel and a ferroelectric gate is one of the emerging approaches due to its potential advantages such as high speed, low power consumption, high density and non-volatility. In an all-oxide based FeFET, $BaSnO_3$ represents one of the most promising semiconducting materials due to its very high carrier mobility which is about 300 $cm^2V^{-1}s^{-1}$ at a carrier density of $8{\cdot}10^{19}$ cm^{-3} [1]. A two-dimensional electron gas (2DEG) will be realized by utilizing a $LaInO_3/BaSnO_3$ interface consisting of polar $LaInO_3$ and non-polar $BaSnO_3$. Within a subproject of the Leibniz Competition project "BaStet" $LaInO_3/BaSnO_3/SrTiO_3$ heterostructures are deposited with the aim to control the charge carrier density of the emerging 2DEG by a ferroelectric $(K,Na)NbO_3$ film by switching its polarization state.

High-quality thin films are essential to achieve such high carrier mobility in La-doped $BaSnO_3$ films. This means especially phase pure films with a low defect density, which can best be obtained by homoepitaxial growth. Since up to now, growth of $BaSnO_3$ single-crystals remains challenging we mainly utilized commercially available $SrTiO_3$ substrates to grow La-doped $BaSnO_3$ films. However, the lattice mismatch between $SrTiO_3$ and $BaSnO_3$ is 5.6% which promotes the formation of a high density of threading dislocations, which again deteriorates electric properties. In 2019, we established a close collaboration with Kookrin Char at Seoul National University, who visited the IKZ for several months during that year. He and his group had been very successful in the research of $BaSnO_3$ films grown by pulsed laser deposition (PLD) and optimized such films with respect to phase purity and high carrier mobility. During that time, a growth routine for the deposition of highly La-doped $BaSnO_3$ films grown on $SrTiO_3$ substrates was developed for the PLD setup used at IKZ. These works are performed in the framework of a master thesis at IKZ (R. Ravindran). First, we optimized the growth conditions to establish the formation of only a single $BaSnO_3$ phase, followed by optimizing the charge carrier mobility of the films. Therefore, 4% La-doped $BaSnO_3$ films were deposited at different laser energies, target-substrate distances and substrate temperatures. The film properties could be optimized to a phase pure 115 nm thick $BaSnO_3$:La film with a carrier mobility of 47 $cm^2V^{-1}s^{-1}$ at a carrier density of $4.3{\cdot}10^{20}$ cm^{-3}.

Fig. 1
X-ray reciprocal space mappings of $BaSnO_3$ heterostructures
(a) with and
(b) without $SrSnO_3$ buffer layer in vicinity of the (444) Bragg reflection of the $NdScO_3$ substrate. The location of bulk $BaSnO_3$ and $SrSnO_3$ peaks are indicated by crosses.



During a two month research stay of PhD student D. Pfützenreuter at Seoul National University, we could make use of the unique advantage of IKZ to provide bulk oxide materials with a large available range of lattice parameters. Hence, for the epitaxial growth of the $BaSnO_3$ thin films we used $NdScO_3$ substrates, which have an average lattice mismatch to $BaSnO_3$ of only 2.7% and thus are expected to result in a lower density of dislocations. First experiments were performed on 50 nm thick 1% La-doped $BaSnO_3$ films grown on a 120 nm thick undoped $BaSnO_3$ buffer layer. Unexpectedly, we detected a rather high defect density compared to films grown on $SrTiO_3$ substrates. We attribute this high density of threading dislocations to the orthorhombic symmetry of the $NdScO_3$, which is in contrast to the cubic symmetry of $SrTiO_3$ and $BaSnO_3$, and causes additional lattice distortions and most likely rotational variants in the films. To overcome the orthorhombic distortion, the 120 nm thick undoped $BaSnO_3$ layer is split into 60 nm thick $SrSnO_3$ and 60 nm thick $BaSnO_3$ buffer layers. $SrSnO_3$ is nearly lattice matched to the $NdScO_3$ substrate and has – in contrast to the $NdScO_3$ substrate – a quasi-cubic unit cell with lattice parameters a = 4.035 Å and b = c = 4.033 Å. Hence we do not expect an orthorhombic distortion of the $BaSnO_3$ layer and thus improved electric properties. By means of reciprocal space mappings we could show that the $SrSnO_3$ buffer layer is almost fully strained on the $NdScO_3$ substrate, while the $BaSnO_3$ and $BaSnO_3$:La layers are partially relaxed. The corresponding reflection peaks are much sharper then the $BaSnO_3$ contribution when directly grown on $NdScO_3$ (compare Fig. 1). The structural improvement is followed by a tremendous electrical improvement confirmed by Hall-measurements, where we determined a carrier mobility of 35 $cm^2V^{-1}s^{-1}$ at a carrier density of $9.2 \cdot 10^{20}$ cm^{-3} for the 50 nm thick La-doped $BaSnO_3$ top layer. From such results we conclude that not only the difference in the lattice parameters is relevant for the formation of defects in the film, but also the symmetry mismatch between film and substrate material.

With the purpose to create a 2DEG at the $LaInO_3$/$BaSnO_3$ interface [2], heterostructures containing five different layers have been deposited (see Figure 2). On top of the $SrSnO_3$ and undoped $BaSnO_3$ buffer layers a 12 nm $BaSnO_3$ film (channel layer) with variable La doping concentration (up to 0.4%) is grown followed by the growth of highly doped $BaSnO_3$ top contacts through a stencil mask. The last step is the deposition of the 10 nm $LaInO_3$ top layer. We observed that at a doping level of at least 0.35 % the conductance of the La-doped $BaSnO_3$ channel layer increased by four orders of magnitude after the deposition of $LaInO_3$, which is a clear indication for the formation of a conductive interface.

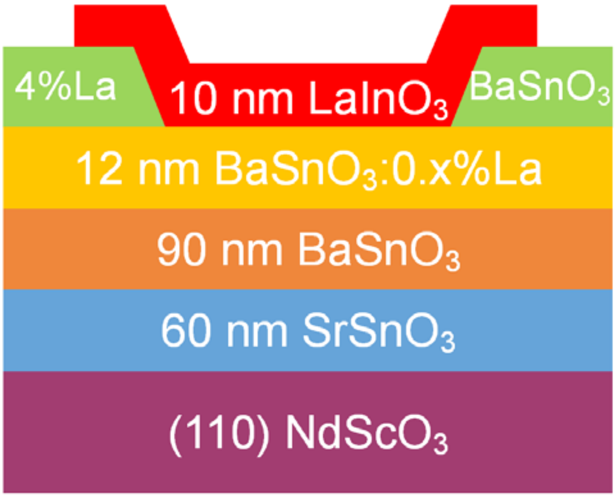


Fig. 2
Schematic heterostructure of the grown 2DEG samples with varying $BaSnO_3$:La channel layer doping concentration.

In summary, we conclude that the approach of using $NdScO_3$ as substrate material, which exhibits a remarkably lower lattice mismatch to $BaSnO_3$ than the typically used $SrTiO_3$ substrate, for $BaSnO_3$ based heterostructures is very promising in terms of electrical and structural properties and the creation of a 2DEG at the $LaInO_3$/$BaSnO_3$ interface. By the use of an additional buffer layer to avoid defects based on the symmetry mismatch between film and substrate, we have confirmed the formation of a conductive $LaInO_3$/$BaSnO_3$ interface. This successful result has been made possible by the close cooperation with K. Char at Seoul National University and the contributions of mutual expertise of both partners.

References

[1] H. J. Kim, U. Kim, H. M. Kim, T. H. Kim, H. S. Mun, B.-G. Jeon, K. T. Hong, W.-J. Lee, C. Ju, K. Hoon Kim, K. Char; *High Mobility in a Stable Transparent Perovskite Oxide.* Appl. Phys. Express 5, 061102 (2012), https://doi.org/10.1143/APEX.5.061102

[2] Y.M. Kim, T. Markurt, Y. Kim, M. Zupancic, J. Shin, M. Albrecht, K. Char; *Interface polarization model for a 2-dimensional electron gas at the $BaSnO_3$/$LaInO_3$ interface.* Sci Rep 9, 16202 (2019), https://doi.org/10.1038/s41598-019-52772-8

The challenge to grow modulation-Si doped ß-Ga_2O_3 multilayers by MOVPE

A. Popp, S. Bin Anooz, R. Grüneberg, A. Fiedler, Z. Galazka, R. Schewski, M. Albrecht, K. Irmscher, and G. Wagner

Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Modern society relies on a wide range of electrical and electronic systems. About 80% of them require the conversion of primary electricity into another form of electricity. Thus, the conversion of electrical energy must be carried out as efficiently as possible. The material system beta-gallium oxide (β-Ga_2O_3) is an emerging ultra-wide bandgap (4.8 eV) [1] semiconducting oxide which is characterized by a theoretical breakdown field strength of 8MV/cm [2]. Due to these properties β-Ga_2O_3 has the potential to outperform SiC and GaN and to become the next generation of high-performance material for power electronic applications. For example: transistors based on β-Ga_2O_3 benefit from a low on-resistance at a given breakdown voltage. This leads to less power losses within a transistor switching operation [3]. The electrically active part of the device is made up of a homoepitaxial thin layers grown by different growth techniques with thicknesses ranging from 10 nm to 5 mm. Recently, we have investigated the effect of growth parameters, substrate miscut angle and the type of doping on the surface morphology and electrical properties of homoepitaxial β-Ga_2O_3 grown by MOVPE [4-6]. Through these process development we try to achieve the predicted material properties to pave β-Ga_2O_3 the way into power electronics. The wafers, which serve as substrates for the epitaxy, are produced from in-house grown crystals made by the group Oxides/Fluorides at IKZ. Two inch diameter bulk β-Ga_2O_3 single crystals were grown by using the Czochralski method [7] to prepare (100) oriented wafers, while (010) oriented wafers were supplied by Tamura Corp., Japan (grown by the EFG method).

From a practical point of view, since the (100) plane is the preferred cleavage plane of β-Ga_2O_3 with the lowest surface energy and easily to be prepared, (100) β-Ga_2O_3 substrates appear to be most adequate for use in electronic devices requiring smooth surfaces, high mobility and a comparatively high growth rate.

Another critical aspect is the miscut of the substrate surface. Previously, we found that the growth on the (100) plane without or with only a small substrate miscut is characterized by a 2D island nucleation growth mode. Double positioning of Ga adatoms induces the formation of twin lamellae that impair the electrical transport properties of the films. By introducing an appropriate miscut of 6°, the terrace width became small enough and comparable to the diffusion length of ad-atoms on the surface which in turn enabled stable step-flow growth on the (100) plane of β-Ga_2O_3. However, the direction of the misorientation must be considered here. While predominantly bilayer steps and two dimensional island growth are found for miscut towards [001], monolayer steps are present for the miscut towards [$00\bar{1}$] despite the same miscut angle of 6°. This has a substantial influence on the quality of the oxide layers [4,5].

On the other hand, the requirements of modern devices can be met by multilayer structures with different doping regimes. Therefore, we developed the process to deposit modulation Si-doped layer structures on (010) and (100) oriented substrates. High structural perfection, a smooth surface morphology and a low defect density of the epi-layer are crucial to achieve the best electrical properties. Another important factor for the device performance are the interfaces between the substrate and layers, and especially between the single doped epi layers. Figure 1 shows the comparison of the morphologies and Si-depth profiles for a multilayer structure grown on a (010) oriented substrate and a (100) 6° off oriented substrate.

The layer grown on the (010) oriented substrate shows in the AFM image elongated two dimensional islands, indicating a faceted surface morphology with a roughness of about 800 pm. The SIMS Si-depth profile for the multilayer grown on the (010) substrate shows a gradual transition from high (HD) to the low Si doped (LD) regions. This seems to be connected to the surface morphology. For the faceted (010) layer surface the incorporation of Si seems to be inhomogeneous resulting in blurred interfaces. A gradual transition of the doping regimes between layers will result in scattering of free charge carries that leads to a decrease of the carrier mobility and overall device performance.

Nanostructures & Layers

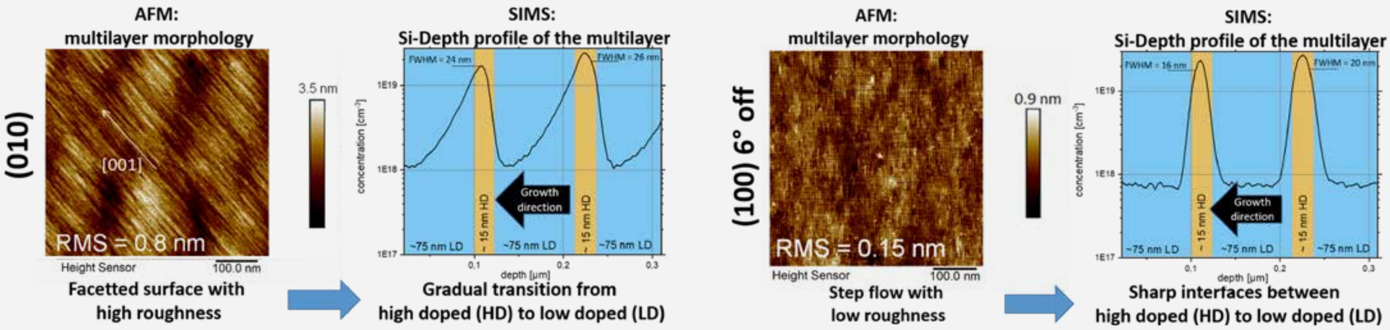


Fig. 1
AFM of the morphology and corresponding SIMS Si depth profile of the multilayer grown by MOVPE on a (010) oriented substrate and a (100) 6° off oriented substrate.

Therefore, it is crucial to ensure that the interfaces are as sharp as possible. This depends strongly on the orientation of the β-Ga_2O_3 substrate. The layer grown on (100) 6° off oriented substrate has a good prerequisite to achieve very sharp interfaces for multilayer structures with different doping regimes. As shown in Figure 1, the morphology measured by AFM is characterized by a smooth step flow growth with a surface roughness of < 200 pm, a quarter the value of the (010) layer. The Si depth profile of the multilayer grown on (100) 6° off substrate shows sharp interfaces between the high and low doping regions. The reason seems to be that the (100) orientation is a cleavage plane with the lowest surface energy [5]. The use of (100) oriented substrates may, therefore, reduce the leakage current and improve the device performance, pointing out a direction for the device development.

In summary, Si-doped β-Ga_2O_3 multilayer structures homoepitaxially grown by MOVPE on (100) oriented substrates revealed smoother morphologies and sharper interfaces in the Si-depth profile compared to (010) oriented substrates. This indicates a prioritized use of (100) oriented substrates for device development due to possible less leakage currents.

Acknowledgment

The content of this report was published as extended abstracts within the frame of the DKT-2020.

This work was performed in the framework of GraFOx, a Leibniz ScienceCampus. The work was partially funded by the BMBF under grant number 03VP03712, the European Community (European Regional Development Fund ERDF) under grant number 1.8/15 and by the Air Force Office of Scientific Research under award number FA9550-17-1-0279.

References

[1] H. H. Tippins; *Optical Absorption and Photoconductivity in the Band Edge of β-Ga_2O_3*, Phys. Rev. **140**, A316 (1965)

[2] M. Higashiwaki, K. Sasaki, H. Murakami, Y. Kumagai, A. Koukitu, A. Kuramata, T. Masui and S. Yamakoshi; *Recent progress in Ga_2O_3 power devices*, Semicond. Sci. Technol. **31**, 034001 (2016)

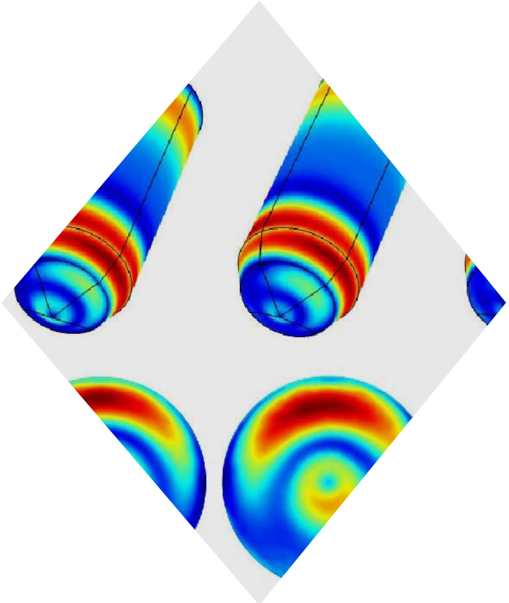
[3] K. Tetzner, E. B. Treidel, O. Hilt, A. Popp, S. Bin Anooz, G. Wagner, A. Thies, K. Ickert, H. Gargouri, and J. Würfl; *Lateral 1.8 kV β -Ga_2O_3 MOSFET with 155 MW/cm^2 Power Figure of Merit,* IEEE Electr. Device L. **40**, 1503 (2019)

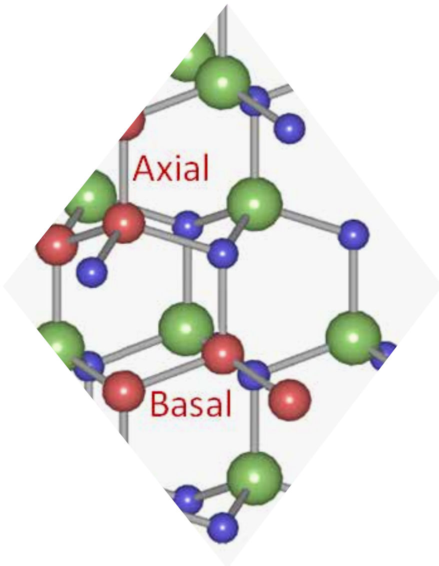
[4] A. Fiedler,R. Schewski, M. Baldini, Z. Galazka, G. Wagner, M. Albrecht, and K. Irmscher; *Influence of incoherent twin boundaries on the electrical properties of β-Ga_2O_3 layers homoepitaxially grown by metal-organic vapor phase epitaxy,* J. Appl. Phys., **122**, 165701 (2017)

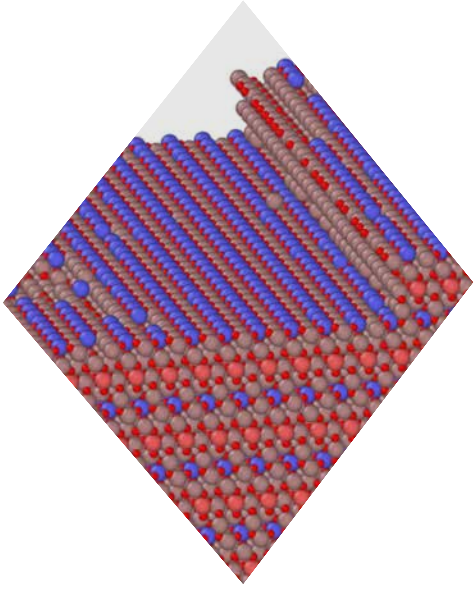
[5] R. Schewski, K. Lion, A. Fiedler, C. Wouters, A. Popp, S. V. Levchenko, T. Schulz, M. Schmidbauer, S. BinAnooz, R. Grüneberg, Z. Galazka, G. Wagner, K. Irmscher, M. Scheffler, C. Draxl, and M. Albrecht; *Step-flow growth in homoepitaxy of β-Ga_2O_3 (100) – The influence of the miscut direction and faceting,* APL Mater. **7**, 022515 (2019)

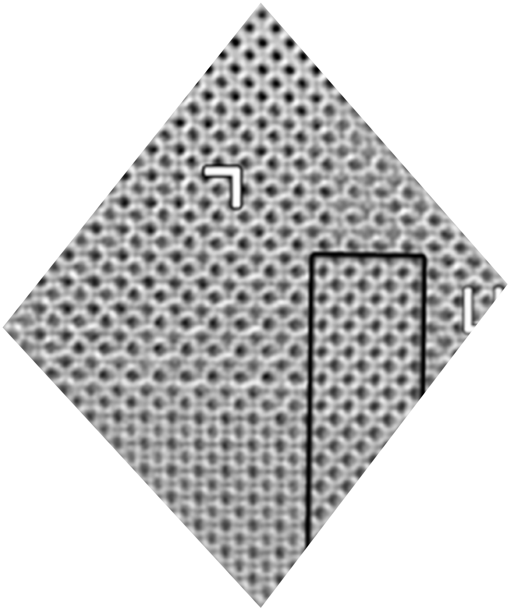
[6] S. Bin Anooz, R. Grüneberg, C. Wouters, R. Schewski, M. Albrecht, A. Fiedler, K. Irmscher, Z. Galazka, W. Miller, G. Wagner, J. Schwarzkopf, and A. Popp; *Step flow growth of β-Ga_2O_3 thin films on vicinal (100) β-Ga2O3 substrates grown by MOVPE,* accepted Appl. Phys. Lett. **116 (2020)**

[7] Z. Galazka; *β-Ga2O3 for wide-bandgap electronics and optoelectronics,* Semicond. Sci. Technol., **33**, 113001 (2018)









Materials Science

Carbon in AlN and GaN: a common dopant incorporating in different atomic configurations

I. Gamov[1], C. Hartmann[1], J. Wollweber[1], A. Dittmar[1], T. Straubinger[1], M. Bickermann[1], I. Kogut[2], H. Fritze[2], E. Richter[3], M. Weyers[3], G. Gärtner[4], F.C. Beyer[5], F. Zimmermann[5], and K. Irmscher[1]

[1]1 Leibniz-Institut für Kristallzüchtung, Berlin, Germany
[2] Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Germany
[3] Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin, Germany
[4] Institute of Experimental Physics, TU Bergakademie Freiberg, Germany
[5] Institute of Applied Physics, TU Bergakademie Freiberg, Germany

Semiconductor crystals of high structural perfection and controlled electrical characteristics are prerequisite to the manufacture of electronic devices from them. In particular, it is necessary to find out how the material can be doped in a controlled manner. Not only the selection of suitable dopants plays a role, but also the formation of compensating point defects, including the introduction of unwanted impurities, must be understood. For this purpose, it is fundamental to identify the defects' chemical nature and atomic arrangement. Unambiguous evidence in this respect can be gained by spectroscopy of local vibrational modes (LVMs) using Fourier transform infrared absorption (FTIR) or Raman scattering techniques.

We have applied these techniques to unintentionally and intentionally C doped AlN crystals grown by physical vapor transport (PVT) at our institute as well as GaN crystals grown by hydride vapor phase epitaxy (HVPE) by our cooperation partners at Ferdinand-Braun-Institut (FBH). Carbon is known by experiment and theory to introduce acceptor levels within the band gaps of these crystals. While in the ultra-wide band gap of AlN of about 6 eV the acceptor level is supposed to be located about 2 eV above the valence band maximum, in the band gap of GaN of about 3.4 eV this level is about 1 eV above the valence band maximum. Hence, in both cases C doping does not contribute to *p*-type conduction at room temperature, but compensates donor dopants. C doping is used in GaN-based high-power device technology to grow buffer layers by metalorganic vapor phase epitaxy for the isolation of device regions from parasitic conductive channels, and in the growth of bulk crystals by HVPE for the preparation of semi-insulating substrates. Both applications are of interest at FBH. In AlN crystals C impurities deteriorate the optical transparency in the deep ultraviolet range where the crystals are intended to be used as substrates for the fabrication of optoelectronic devices.

Therefore, the incorporation of C in AlN during the crystal growth by PVT must be suppressed as much as possible and belongs to the subjects we elaborate at IKZ in the project AlN-230nm within the BMBF funded consortium „Advanced UV for Life“. Contrary, the application of AlN in piezoelectric devices operating at high temperatures needs material that maintains high electrical resistivity at temperatures above 1000°C to reduce electro-mechanical losses, which may be obtained by controlled increase of C incorporation during crystal growth. This is an issue that is treated in cooperation with colleagues from TU Clausthal, DFG project BI 781/11.

Currently, a single carbon atom substituting for a nitrogen host atom (C_N) is considered the pre- vailing defect that is caused by C doping in AlN and GaN. C_N possesses the above-mentioned deep acceptor levels and has low formation energy compared to other carbon-related defects. In addition, C_{Ga} (carbon on gallium site), C_i (interstitial carbon), and various carbon-related complexes with intrinsic defects or other impurities such as hydrogen, oxygen, or silicon have been discussed, and due to their action as donors or (partly passivated) acceptors, they may be involved in the compensation process. Among the defect complexes consisting of multiple carbon atoms only for carbon pairs theoretical predictions are available which report high to moderate pair formation energies making substantial defect concentrations under thermodynamic equilibrium conditions less probable.

However, we recently identified di- and tri-carbon defects in AlN as well as tri-carbon defects in GaN. The proof of the defects' nature is based on an analysis of LVMs observed in Raman scattering or infrared absorption spectra of crystals containing carbon in natural isotopic and ^{13}C isotope enriched composition.

Materials Science

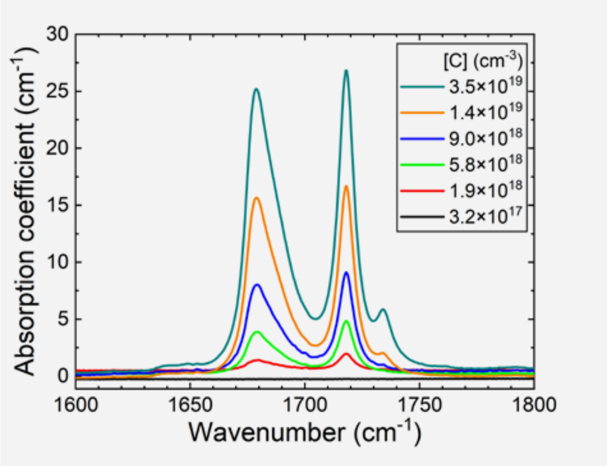


Fig. 1
Room-temperature FTIR spectra of GaN crystals grown by HVPE and doped with carbon of natural isotopic composition

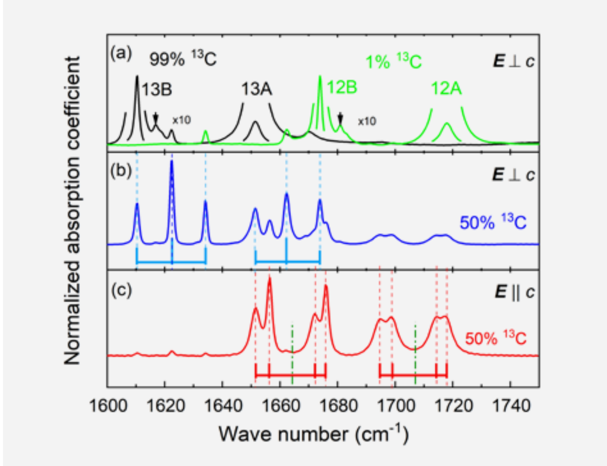


Fig. 2
Low-temperature FTIR spectra illustrating the isotope effect (a) in GaN samples containing C in natural isotopic composition (1% ^{13}C, 99% ^{12}C) and strongly ^{13}C enriched composition (99% ^{13}C, 1% ^{12}C) as well as (b) and (c) in a sample of equal content of both C isotopes (50% ^{13}C, 50% ^{12}C) for perpendicular and parallel polarization of the incident light respectively.

Here we shortly sketch this analysis for the tri-carbon defect in GaN. FTIR spectra of GaN samples doped with C of the natural isotopic composition (~1% ^{13}C, ~99% ^{12}C) are shown in Fig. 1 in the wavenumber region above the strong absorptions of the reststrahlen band and two-phonon-combination bands. They reveal two prominent absorption lines at 1679 cm^{-1} and 1718 cm^{-1} whose intensity increases with the carbon concentration but are visible for carbon concentrations above about 10^{18} cm^{-3} only.

Figure 2a demonstrates that both lines are shifted to lower wavenumbers in a sample doped predominantly with the isotope ^{13}C (99%). Since this shift is fully in agreement with the prediction of the harmonic oscillator model for the exchange of the isotope mass of ^{12}C by that of ^{13}C, we assign the absorption lines to local vibrational modes than to electronic transitions. The spectra of a sample containing both C isotopes in equal portions (50% ^{13}C, 50% ^{12}C), see Figs. 2b and 2c, reveal the appearance of additional lines. Number, spectral positions, and intensities of the LVMs we can consistently interpret on the basis of the harmonic oscillator model considering the probability of possible isotope combinations. Including the polarization dependence of the LVM absorption, we show that the tri-carbon defects form a triatomic molecule-like structure in two crystallographically different configurations: a basal configuration with the carbon bonds near the basal plane and an axial configuration with one of the carbon bonds along the c axis as shown in Fig. 3. Finally, the disappearance of the LVMs under additional below-bandgap illumination is interpreted as defect recharging, i.e., the tri-carbon defects possess at least one charge state transition level within the bandgap and contribute to optical absorption as well as to the electrical charge balance. A rough concentration estimation for the tri-carbon defects suggests substantial concentrations exceeding those of other carbon related defects at carbon doping levels of 10^{19} cm^{-3}. Our investigations show that di- and tri-carbon defects must be included in any reliable interpretation of the electrical and optical properties of moderately to highly C doped GaN and AlN.

Fig. 3
Model of the tri-carbon C_N–C_{Ga}–C_N defect in GaN in the two crystallographically inequivalent configurations.

Publications

[1] I. Gamov, E. Richter, M. Weyers, G. Gärtner, and K. Irmscher; *Carbon doping of GaN: Proof of the formation of electrically active tri-carbon defects*, J. Appl. Phys. **127**, 205701 (2020).

[2] I. Gamov, C. Hartmann, J. Wollweber, A. Dittmar, T. Straubinger, M. Bickermann, I. Kogut, H. Fritze, and K. Irmscher; *Carbon pair defects in aluminum nitride*, J. Appl. Phys. **126**, 215102 (2019).

[3] I. Kogut, C. Hartmann, I. Gamov, Y. Suhak, M. Schulz, S. Schröder, J. Wollweber, A. Dittmar, K. Irmscher, T. Straubinger, M. Bickermann, and H. Fritze; *Electromechanical losses in carbon- and oxygen-containing bulk AlN single crystals*, Solid State Ionics **343**, 115072 (2019).

[4] E. Richter, F.C. Beyer, F. Zimmermann, G. Gärtner, K. Irmscher, I. Gamov, J. Heitmann, M. Weyers, and G. Tränkle; *Growth and Properties of Intentionally Carbon-Doped GaN Layers*, Cryst. Res. Technol. **55**, 1900129 (2020).

Materials Science

Kinetic Monte Carlo simulations for the homoepitaxial growth of β-Ga_2O_3

W. Miller, A. Popp, R. Schewski, S. Bin Anooz, and M. Albrecht

Leibniz-Institut für Kristallzüchtung, Berlin, Germany

ß-Ga_2O_3 is an excellent candidate for power electronics and optoelectronic applications [1]. Since some time it has been one focus of research at IKZ, bulk crystal growth as well as by metal organic vapour phase epitaxy (MOVPE). Epitaxial growth of ß-Ga_2O_3 is a main step towards devices, because the epitaxial layer acts as the functionalpart. However, the epitaxial growth is not yet fully understood and it is highly desirable to support experimental investigations by numerical calculations. Kinetic Monte Carlo (KMC) is a typical method to mimic the kinetic processes during growth. The key point is to define the relevant processes such as adsorption, diffusion, and desorption. We defined these processes on the basis of a series of experiments in the group "semiconducting oxide layers" and detailed analysis by scanning transmission electron microscope (STEM) in the group "electron microscopy". We consider only MOVPE on (100) planes, since it was the only surface where step growth has been achieved so far [2–4]. In particular we set up a KMC model, which reflects the structure of Ga_2O_3 with its 8 Ga atoms and 20 O atoms in the unit cell.Ga and O_2 can adsorb. The sticking coefficient is set according to the local environment. Ga and O atoms can diffuse, also clusters of Ga and O can diffuse in **c**-direction. There is evidence from experiments that Ga_2O can desorb and thus, we consider this in KMC. We make a list of all possible events with their probabilities and chose in every iteration one event randomly with respect to its relative probability to the sum of probabilities of all events. The diffusion energies were set in the range of 1.5 eV because a 1D mean field approach for island growth gave a value of this order by comparison with experimental results [3].

Firstly, we performed runs for a flat surface. STEM HAADF images of the surfaces reveal that the terraces are always B1 or B2-plane (see Fig. 1) [5]. One critical parameter is the O/Ga ratio of atoms arriving at the surface. For small O/Ga ratio no critical nucleus could be formed. The larger the ratio the faster the growth. Nevertheless, no 3D growth is observed but first the next B-plane is filled up. This corresponds with the experimental observations. Choosing a fixed ratio we performed runs for 750°C, 800°C, and 850°C. For the latter we observe large 2D islands as in the experiments. At lower temperature the growth is faster but structures are smaller.

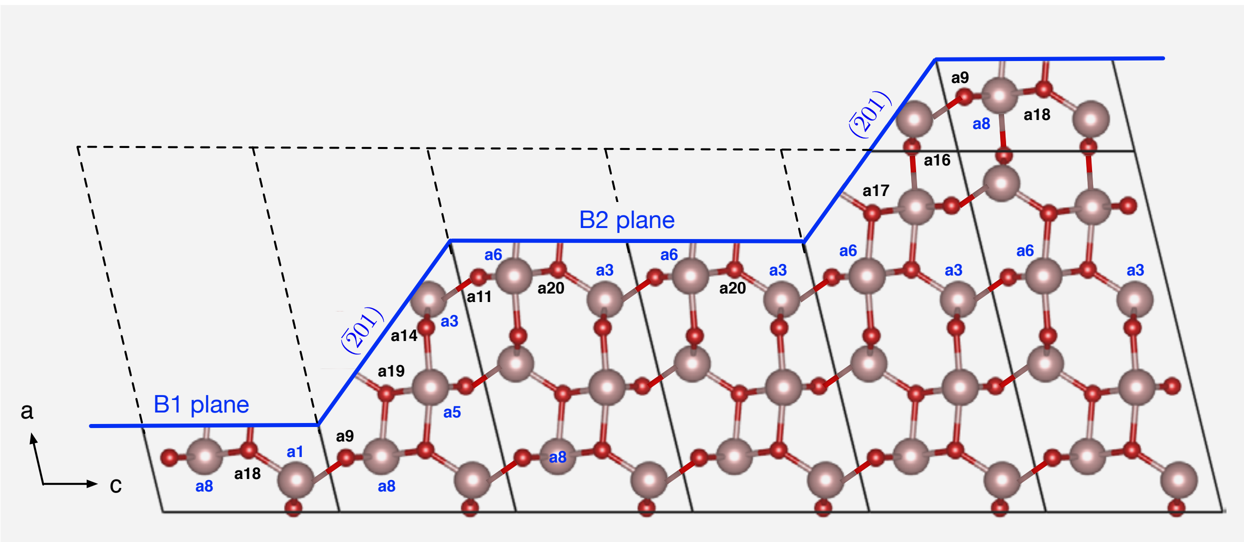


Fig. 1
Surface planes as observed in the STEM analysis. Atoms are labeled according to their number in the KMC code.

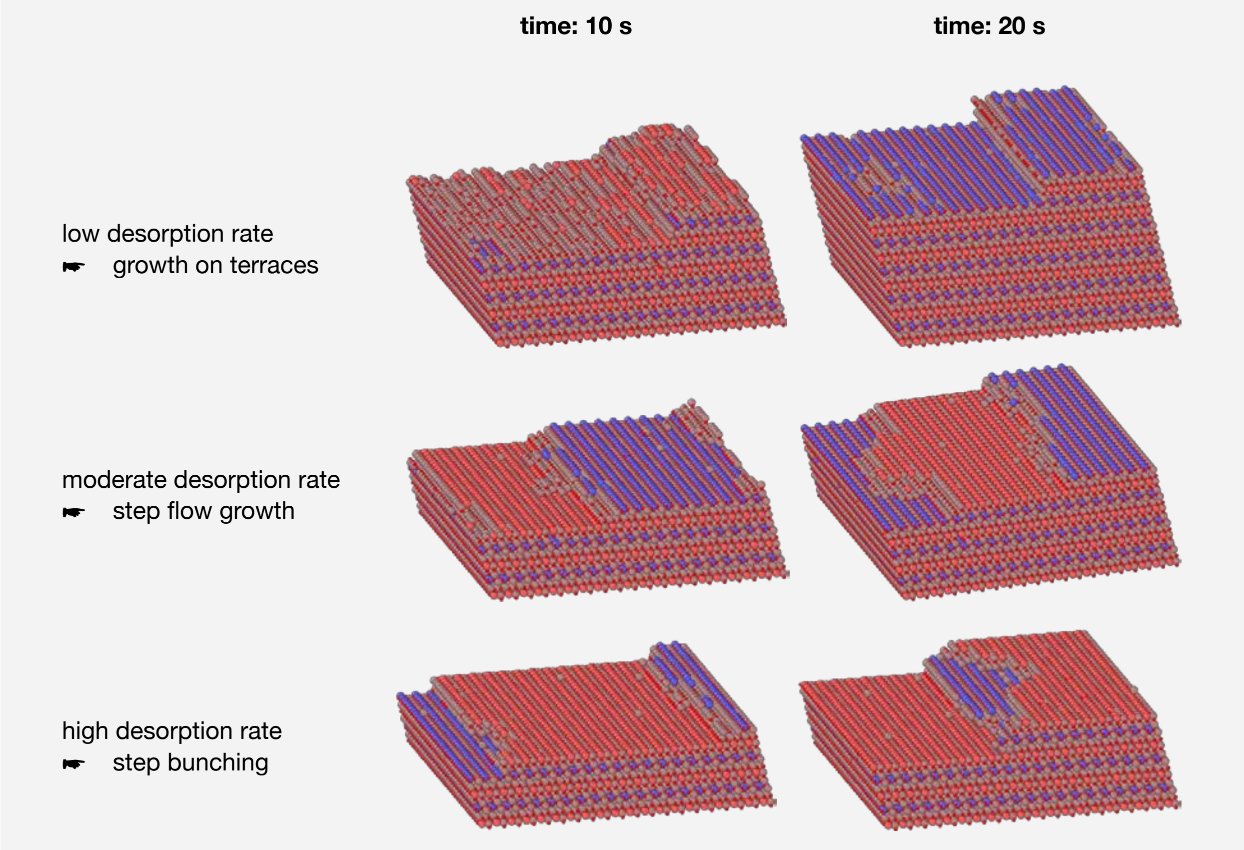


Fig. 2
Surface morphologies for runs with different desorption rates. Light red atoms: Ga atoms at top of B1 plane. Blue atoms: Ga atoms at top of B2 plane. Grey atoms: other Ga atoms. Red atoms: oxygen.

On order to grow layers of high quality one likes to have a step flow growth. Therefore, to avoid double positioning which results in twin lamellae and finally in 2D island growth, vicinal (100) surfaces with a 6° miscut towards the [00-1] direction were provided [6]. Here we study the influence of the desorption rate, which can be manipulated in the experiment by choosing different chamber pressures. For an intermediate desorption rate (as used for the flat surface) we obtain step growth (case B in Fig. 2). For high desorption rate (case C) we observe step bunching because every fluctuation in edge growth leads to a growth instability. In the opposite case (case A) we observe chaotic growth on the terraces but eventually ending up in a double step. The final morphology looks similar to that of case C. Please note that we have only two steps in our KMC run and cannot make any realistic statement beyond the 20 s shown in Fig. 2. The results have been submitted for publication. Currently, we develop a phase field model to treat larger domains with several steps.

Acknowledgement

This work was partially conducted in the frame of Science Campus for Growth and Fundamentals of Oxides (GraFox) supported by the Leibniz Association.

References

[1] M. Higashiwaki, H. Murakami, Y. Kumagai, A. Kuramata, *Current status of Ga_2O_3 power devices*, Jap. J. Appl. Phys., 55, 1202A1 (2016).

[2] T. Oshima, N. Arai, N. Suzuki, S. Ohira, S. Fujita, *Surface morphology of homoepitaxial β-Ga_2O_3 thin films grown by molecular beam epitaxy*, Thin Solid Films, 516, 5768 (2008).

[3] R. Schewski, M. Baldini, K. Irmscher, A. Fiedler, T. Markurt, B. Neuschulz, T. Remmele, T. Schulz, G. Wagner, Z. Galazka, *Evolution of planar defects during homoepitaxial growth of β-Ga_2O_3 layers on (100) substrates-A quantitative model*, J. Appl. Phys., 210, 225308 (2016).

[4] M.-Y. Tsai, O. Bierwagen, M. E. White, J. S. Speck, *β-Ga_2O_3 growth by plasma-assisted molecular beam epitaxy*, J. Vac. Sci. Technol. A 28, 354 (2010).

[5] P. Voigt, O. Bierwagen, *Reaction kinetics and growth window for plasma-assisted molecular beam epitaxy of β-Ga_2O_3: Incorporation of Ga vs. Ga_2O desorption*, Appl. Phys. Lett. 109, 062103 (2016).

[6] R. Schewski, K. Lion, A. Fiedler, C. Wouters, A. Popp, S. V. Levchenko, T. Schulz, M. Schmidbauer, S. Bin Anooz, R. Grüneberg, *step-flow growth in homoepitaxy of β-Ga_2O_3(100)-The influence of the miscut direction and faceting*, APL Mater., 7, 022515 (2019).

Materials Science

Interface polarization model for a 2-dimensional electron gas at the $BaSnO_3$/$LaInO_3$ interface

M. Zupancic[1], W. Aggoune[2], T. Markurt[1], Y. M. Kim[3], Y. Kim[3], J. Shin[3], K. Char[3], C. Draxl[2], and M. Albrecht[1]

[1]Leibniz-Institut für Kristallzüchtung, Berlin, Germany
[2]Institut for Physik and IRIS Adlershof, Humboldt Universität zu Berlin, Germany
[3] Institute of Applied Physics, Dept. of Physics and Astronomy, Seoul National University, Seoul, South Korea

Over the last decade, many studies have focused on polar - non-polar perovskite oxide interfaces due to the potential to realize novel electronic devices, and to tune the electronic phase between metallic, semiconducting and superconducting. The formation of a 2-dimensional electron gas at the interface, as well as the mobility of carriers and other physical properties, crucially depend on the atomic structure of the interface. Since most of these heterostructures are heteromorphous, the orientation relationship between these perovskites is an important issue. In classical group IV semiconductors or III-V compounds, the interface energy in most cases is negligible, and the total energy is dominated by the strain energy. The strain induced by the substrate in these systems is accommodated by the tetragonal distortion of the unit cell and can be calculated by continuum elasticity theory. Epitaxial growth of ABO_3 perovskite oxides on each other is governed by a number of peculiarities:

1: Perovskites in most cases exhibit different crystal symmetry (e.g. perfect cubic, rhombohedral, orthorhombic) mediated by symmetry reducing distortions of the perfect cubic structure, reflected in the respective tilt of the BO_6 octahedra. If e.g. a layer with lower symmetry grows coherently on a substrate with perfect cubic symmetry, different epitaxial relationships are possible.

2: Perovskites can adopt strain by both octahedral rotations (along the surface normal or perpendicular to it) and by relative displacement of cations and anions, i.e. by distortions of the unit cell. Peculiarities of the accommodation will strongly depend on the chemistry of the compound.

3: The interface may play an important role in the energetics of the system. The tilt pattern of the substrate may influence the one of the epitaxial layers and counteract strain accommodation. Chemistry then may control the energy balance instead strain. Another important contribution that controls interface formation is the charge that is present at a polar - non-polar interface.

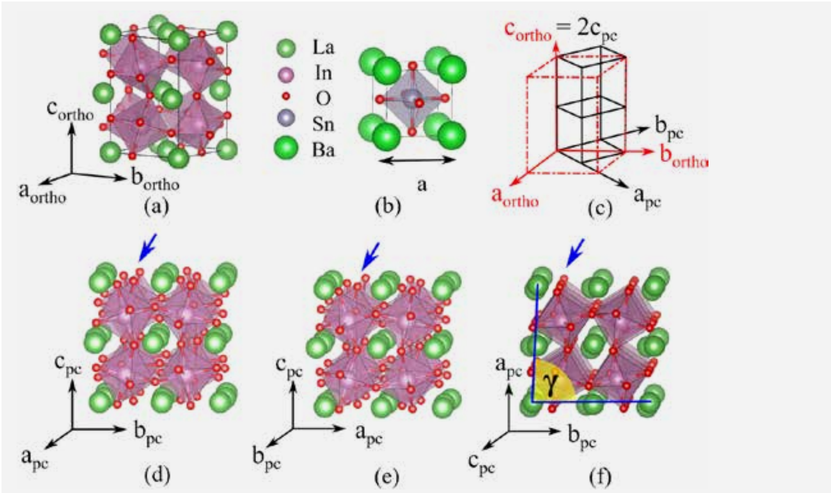


Fig. 1

Sketch of the primitive unit cell of (a) orthorhombic $LaInO_3$ and (b) cubic $BaSnO_3$. (c) Scheme of the epitaxial relationship between the $LaInO_3$ orthorhombic (red) and pseudocubic (black) unit cell. $a^-a^-c^+$ Glazer tilt pattern describes InO_6 octahedral tilt in $LaInO_3$ orthorhombic perovskite structure: (b) a^- out-of-phase tilt around a_{pc} = $[100]_{pc}$ axis (out-of-phase tilt signify oxygen octahedra which rotate along the pseudocubic rotational axis in opposite direction), (c) a^- out-of-phase tilt around b_{pc} = $[010]_{pc}$ axis and (d) c^+ in-phase tilt around c_{pc} = $[001]_{pc}$ axis (in-phase tilt signify oxygen octahedra which rotate along the rotational axis in the same direction). The angle between a_{pc} and b_{pc}, (γ), equals 87.6˚.

In the framework of the project BaStet (Barium stannate based heterostructures for electronic applications) funded by the Leibniz Competition and the Leibniz ScienceCampus GraFOx we explore the interface between $BaSnO_3$ and $LaInO_3$ by an international experimental and theoretical effort of IKZ, Humboldt Universität Berlin, Technical University of Berlin and Seoul National University. $BaSnO_3$ is a perfect cubic wide bandgap perovskite oxide which attracted attention since it exhibits the highest electron mobility (~300 cm^2/Vs) of all known transparent conductive oxides.

The electron mobility remains high even at lanthanum doping concentration of 10^{20} cm^{-3}. When combined in heterostructure with $LaInO_3$ a two-dimensional electron gas (2DEG) is formed. As for the archetypical system $LaAlO_3/SrTiO_3$ the origin of the formation of the 2DEG is still discussed controversially. A common model attributes it to the charge transfer between polar wider bandgap perovskite (here $LaInO_3$) and the non-polar perovskite oxide (here $BaSnO_3$). In our work, performed in collaboration with Kookrin Char from Seoul University, we study the atomic structure of the $BaSnO_3/LaInO_3$ interface and focus on the role of the octahedral tilt at their interface [1]. Fig. 1 summarizes the crystallographic properties of both compounds in terms of the tilt pattern. $LaInO_3$ can grow in three possible epitaxial relations onto $BaSnO_3$ (Fig. 1 (d), (e), and (f). Scheme of the epitaxial relationship between the $LaInO_3$ orthorhombic and pseudocubic unit cell is shown in the Fig. 1 (c). In the following we restrict ourselves to HRTEM data of a_{pc} oriented grains of $LaInO_3$

We quantitatively evaluate the octahedral tilt from exit wave reconstruction obtained from experimental focal series.

Fig. 2(a) shows the amplitude of the exit wave and the corresponding image simulation as an inset. Fig. 2(b) shows that the measured octahedral tilt from the cubic $BaSnO_3$ (no tilt) to the bulk value of $LaInO_3$ gradually changes along few pseudocubic unit cells. At the same time, the out-of-plane lattice parameter shows increases. Modelling of the 2DEG at the interface between $BaSnO_3$ and $LaInO_3$ on experimental inputs such as bandgaps, band offsets and carrier concentration requires the presence of an interface polarization in $LaInO_3$ extending over 2 pseudocubic unit cells to explain the measured carrier concentration at the interface. We hypothesize that the suppression of the octahedral tilt at the interface induces this interfacial polarization.

To understand the physical origin that causes the suppression of the octahedral tilt in $LaInO_3$, we combine the efforts of HRTEM and density functional theory. Based on bulk properties, we expect an γ angle of 90° for $BaSnO_3$ and of 87.6° for $LaInO_3$ in the particular orientation shown in Fig: 1. Close to the interface our measurements however show a γ angle of $LaInO_3$ of 88.9° ± 1°, which is closer to 90° of $BaSnO_3$ than to the expected equilibrium value of $LaInO_3$ of 87.6°. As a reference, we use cubic $BaSnO_3$ where the γ angle equals to 90˚. If we calculate the formation energy for a structure that fixes the y-angle to the bulk value of $LaInO_3$ and compare it to that of a relaxed structure we find an angle of 88.5° close to the experimentally observed one, accompanied by a reduced formation energy for the latter (-2.429 eV/atom instead of 2.419 eV7atom). This change in bond angles is mediated by changes in the In-O bond length and shifts of La atoms in the region close to the interface. We also show that the change of the bond angle in $LaInO_3$ is unfavourable with respect to elastic strain relaxation. This implies that the tilt pattern of $LaInO_3$ at the interface of the $LaInO_3/BaSnO_3$ heterostructure is dominated by the the polar non-polar nature of the interface, and has strong impact on the formation of the 2DEG.

References

[1] Y. M. Kim, T. Markurt, Y. Kim, M. Zupancic, J. Shin, M. Albrecht and K. Char: *Interface polarization model for a 2-dimensional electron gas at the BaSnO3/LaInO3 interface;* Scientific Reports 9, 16202 (2019)

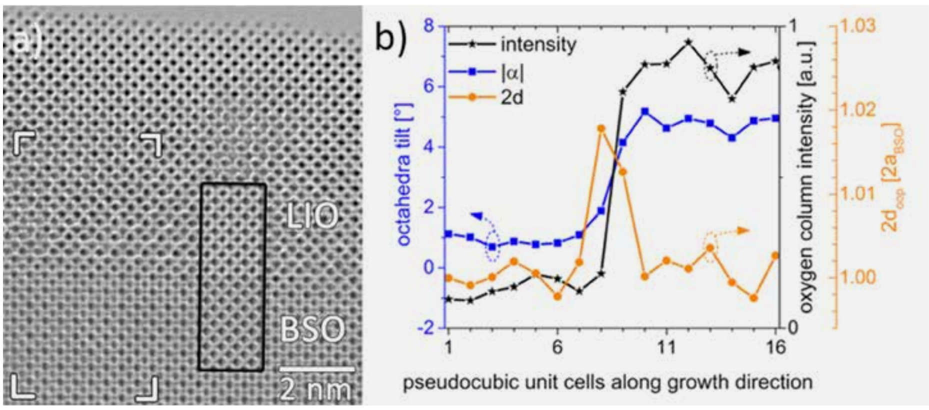


Fig. 2
Octahedral tilt at the interface between $BaSnO_3$ and $LaInO_3$. a) Amplitude of the exit wave with a simulation as an inset (black frame). b) Line profiles across the $BaSnO_3/LaInO_3$ interface of the laterally averaged values of |α| - modulus of the oxygen octahedra tilt, $2d_{oop}$, and the intensity of oxygen atomic columns.

Modelling of the Czochralski growth of neodymium scandate single crystals

K. Böttcher, W. Miller, and S. Ganschow

Leibniz-Institut für Kristallzüchtung (IKZ), Berlin, Germany

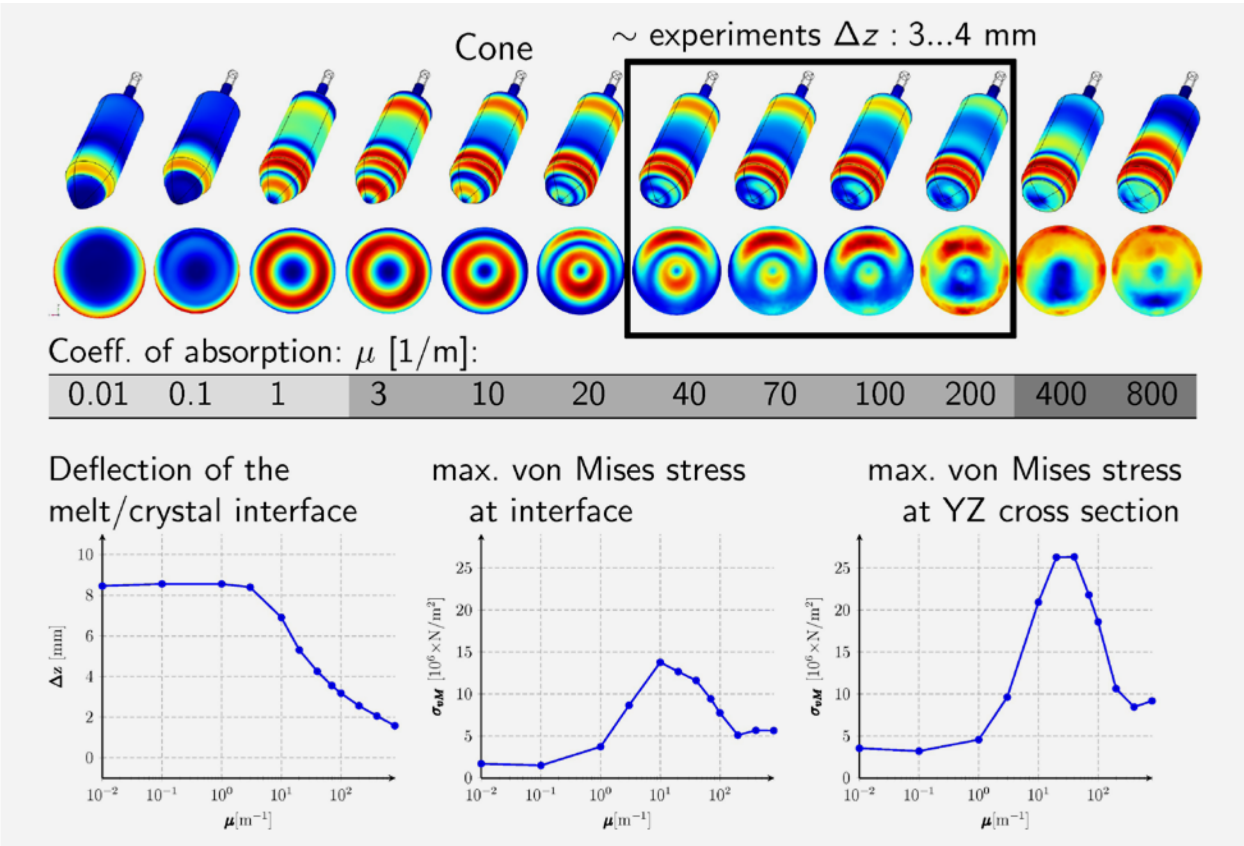


Fig. 1
Top: Von Mises stress at the crystal surface and at the crystal/melt interface (the circle below) as a result of the action of the absorption coefficient (see gray-scaled row from 0.01 … 800 1/m),
Bottom: Some results items in dependence of the absorption coefficient along the full range.

Rare-earth (RE) scandates with RE = La–Ho are excellent substrate materials for the expitaxial growth of high-quality films of a variety of ferroelectric [1,2,3], multiferroic [4,5], and superconducting [6] perovskites. By tempering strain achieved in coherent epitaxial films grown on RE scandates, their ferroelectric properties can be tuned [7]. Among the RE scandates that can be grown using the Czochralski technique, $NdScO_3$ is the material with the largest pseudocubic lattice parameter and marks therefore a corner of the strain-engineering technique.

$NdScO_3$ melts congruently, and single crystals can be grown by the Czochralski method with induction heating and automatic diameter control. Concerning the internal radiative heat transfer, $NdScO_3$ crystals are semitransparent which is a very challenging property to treat numerically. In our investigations we have used the software CGSim™ as a tool for modelling crystal growth from the melt. For solving the radiative transport, CGSim™ uses a variant of the Discrete Transfer Method, which enables to solve the thermal radiation transport for the full range of optical thickness.

The Czochralski growth of $NdScO_3$ crystals with a geometry of up to 45 mm in length and 18 mm in radius marks the present state of the art. However, crystals tend to crack during wafer preparation, for that reason we are interested in the analysis of thermal stresses. In order to handle the radiative heat transfer, as a first approach, we have defined different value ranges of a grey absorption coefficient μ in order to meet the various branches of the dimensionless optical thickness τ: for μ= 0.01 ... 3 m^{-1} we get τ: < 0.1, i.e. the medium is optical thin, for μ= 400... 800 m^{-1} we get τ > 10, i.e. the medium is optical thick, and for μ= 10 ... 200 m^{-1}, the medium is modelled as moderately optical thick. The computations are performed in two steps: Step one is the axisymmetric calculation of the temperature field in the entire furnace and of the velocity field in melt and gas, additionally with power computation relocation of the finite-element mesh in order to track the shape of the crystal/melt interface. In step two, we take geometry and temperature field from the crystal and expand them to 3D by rotating their data along 360 degree. This new data structure is put into software COMSOL here the anisotropic coefficients of thermal expansion and elasticity can be utilized in order to make 3D displacements and thermal stresses in terms of the von Mises stress. Fig. 1 shows the von Mises stress at the crystal surface for the absorption coefficients ranging from optically thin (very left) via intermediate to thick. From the deflections of the crystal/melt interface and the maximum values of the von Mises stress as shown here, we see that the cases with the largest stress values have intermediate absorption. Exactly these data sets have a similar deflection of the crystal/melt interface as in experiments: between 3 and 4 mm. This could explain the large residual stresses which lead to mechanical cracking at wafer preparation. This result is also not affected by the crystal geometry: For those cases (indicated by a frame in Fig. 1) Fig. 2 shows the stress distribution within the crystals along a cross cut plane, for crystals with and without the shoulder next to the seed. The absence of the shoulder does not essentially change the thermal stress distribution near the crystal/melt interface.

References

[1] Haeni, J., Irvin, P., Chang, W., *Room-temperature ferroelectricity in strained $SrTiO_3$,* Nature 430 (2004) 758.

[2] M. D. Biegalski, Y. Jia, D. G. Schlom, S. Trolier-McKinstry, S. K. Streiffer, V. Sherman, R. Uecker, and P. Reiche, *Relaxor ferroelectricity in strained epitaxial $SrTiO_3$ thin films on $DyScO_3$ substrates*, Appl. Phys. Lett. 88 (2006) 192907.

[3] K. J. Choi, M. Biegalski, Y. L. Li, A. Sharan, J. Schubert, R. Uecker, P. Reiche, Y. B. Chen, X. Q. Pan, V. Gopalan, L.-Q. Chen, D. G. Schlom, C. B. Eom, *Enhancement of Ferroelectricity in Strained $BaTiO_3$ Thin Films*, Science 306 (2004) 1005.

[4] A. Vasudevarao, A. Kumar, L. Tian, J. H. Haeni, Y. L. Li, C.-J. Eklund, Q. X. Jia, R. Uecker, P. Reiche, K. M. Rabe, L. Q. Chen, D. G. Schlom, and Venkatraman Gopalan, *Multiferroic Domain Dynamics in Strained Strontium Titanate*, Phys. Rev. Lett. 97 (2006) 257602.

[5] Y. H. Chu, Q. Zhan, L. W. Martin, M. P. Cruz, P. L. Yang, G. W. Pabst, F. Zavaliche, S. Y. Yang, J. X. Zhang, L. Q. Chen, D. G. Schlom, I. N. Lin, T. B. Wu, R. Ramesh, *Nanoscale Domain Control in Multiferroic $BiFeO_3$ Thin Films*, Adv. Mater. 18 (2006) 2307.

[6] S. Karimoto, M. Naito, Electron-doped infinite-layer thin films with T_C over 40 K grown on $DyScO_3$ *substrates*, Appl. Phys. Lett. 84 (2004) 2136.

[7] Darrell G. Schlom, Long-Qing Chen, Chang-Beom Eom, Karin M Rabe, Stephen K Streiffer, and Jean-Marc Triscone, *Strain Tuning of Ferroelectric Thin Films*, Annu. Rev. Mater. Res. 37 (2007) 589.

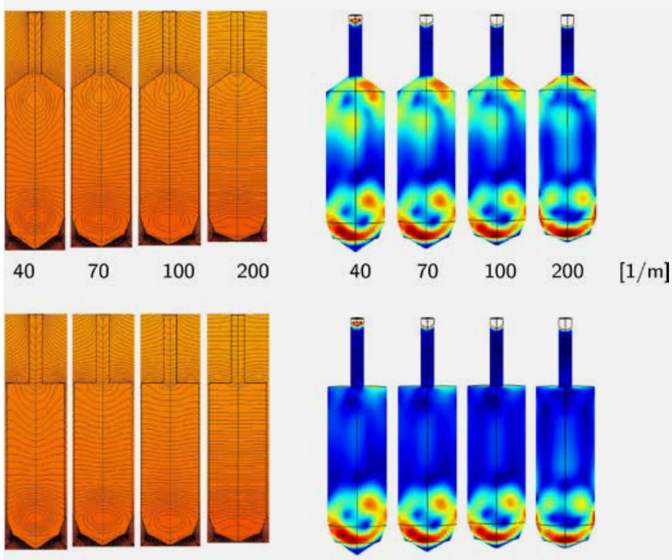
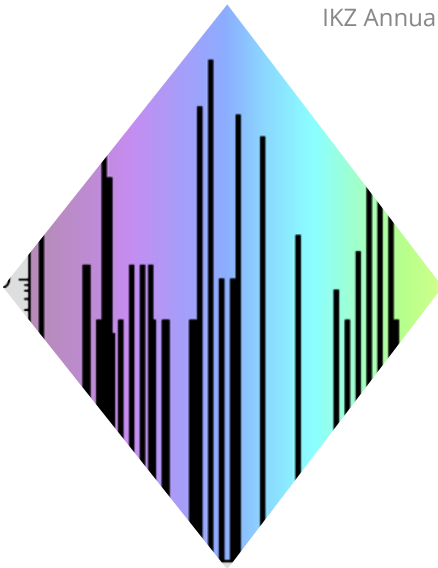
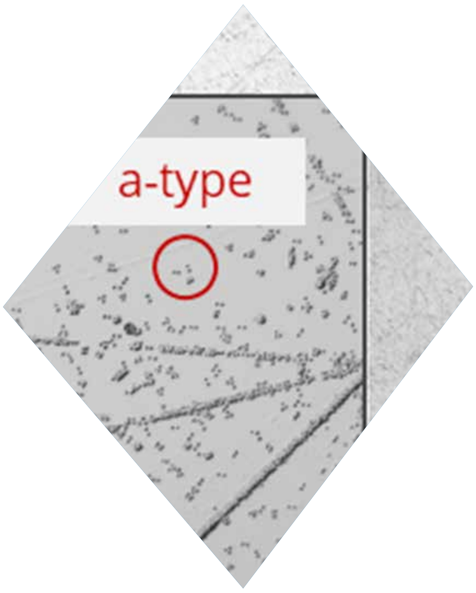


Fig. 2
Top:
Temperature field and von Mises stress at a crystal cross cut for the cases where the crystal/melt interface is in the range of the experimentally observed values:
Top:
Case with crystal shoulder next to the seed,
Bottom: Case without shoulder.





Application Science

Application Science

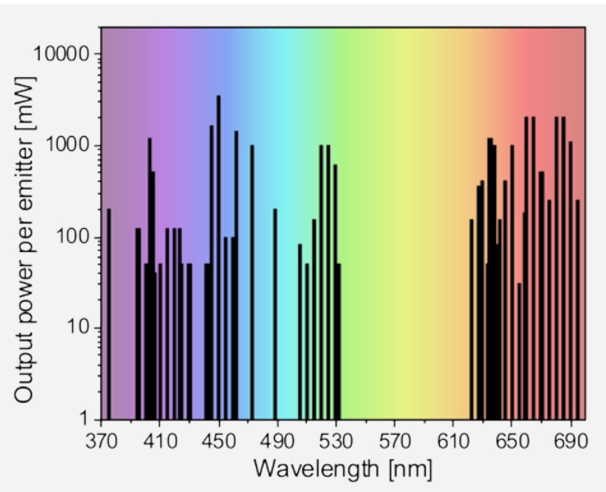
Diode-pumped Tb^{3+}-lasers as a strategy for direct laser emission in the visible range

E. Castellano-Hernández[1], S. Kalusniak[1], P. W. Metz[2], and C. Kränkel[1]

[1] Leibniz-Institut für Kristallzüchtung, Berlin, Germany
[2] Institut für Laser-Physik, Universität Hamburg, Hamburg, Germany

Researchers from the Center for Laser Materials (ZLM) at the IKZ demonstrated the first Tb^{3+}-based diode-pumped solid-state laser (DPSSL). This simple and efficient laser is pumped by an InGaN-laser diode at 488 nm in the blue and emits directly at 545 nm in the green and 587 nm in the yellow spectral range, respectively. In particular the transition at 587 nm is of high relevance, as directly yellow emitting DPSSLs are currently not commercially available.

The immense variety of lasers sources that have been developed in science and industry comes from the necessity to fulfill the specific requirements of medical, industrial, research, and daily life applications. While nearly arbitrary laser parameters can be realized by complex and very expensive multi-stage laser systems, there is an increasing demand for lasers which are simple, easy to handle, compact, and inexpensive. Diode lasers match these characteristics and therefore have been extensively developed in the last decades. Still, up to now it remains an unsolved challenge to develop practical diode sources emitting at wavelengths in the so-called "green gap" extending from ~530 nm to ~620 nm in the visible range, including parts of the green and the whole yellow spectral range. Fig. 1 exhibits the market availability of diode lasers in the visible and exposes the necessity to find alternative laser sources for the "green gap".



Visible laser sources are clearly important for daily life applications such as display technology or entertainment. But there are many less intuitive applications requiring visible laser emission at very specific wavelengths. Lasers at 589 nm are used for excitation of the sodium D-line in spectroscopy as well as for the generation of guide stars for astronomy by excitation of sodium in the upper layers of the atmosphere to correct atmospheric-induced telescope aberrations. In ophthalmology, yellow lasers are better suited than green lasers, which are commonly used due to their better availability. Stronger absorption of hemoglobin in the yellow allows for a reduction of the required power by about one third in comparison to green lasers, decreasing the risk of retinal damage. This feature makes yellow lasers interesting for further medical applications such as skin treatment or flow cytometry.

Currently, laser emission in the yellow is in most cases either based on toxic dye lasers, inefficient copper-bromide vapor lasers, or complex frequency conversion systems. However, in the absence of directly emitting laser diodes at the required wavelength, the most simple and efficient solution would be a DPSSL.

In 2019, researchers from the Center for Laser Materials (ZLM) at the IKZ made an important step in this direction by presenting such a DPSSL directly emitting at wavelengths in the green and yellow range inside the "green gap" [1]. This laser is based on Tb^{3+}-doped fluoride crystals, which had been developed at the ZLM. In their previous work, the ZLM researchers had revealed, that utilizing highly Tb^{3+}-doped crystals enables the most efficient directly yellow emitting solid-state lasers [2]. However, these first reports were utilizing pump sources which were complex and inefficient frequency doubled lasers themselves.

Fig. 1
Output power of commercially available single emitter laser diodes emitting in the visible spectral range [1].

Application Science

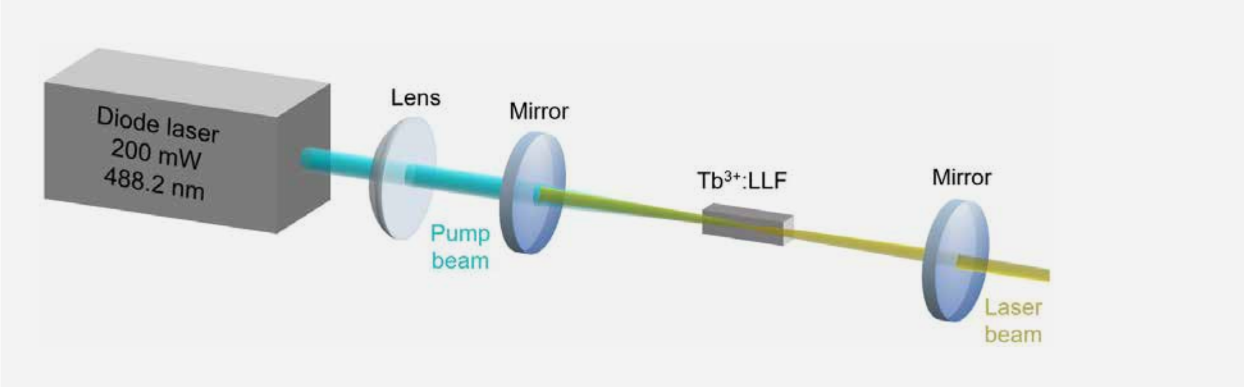


Fig. 2
Sketch of the yellow DPSSL setup.

In their recent research breakthrough, ZLM-researcher Elena Castellano-Hernández and her colleagues demonstrated the suitability of modern blue-emitting laser diodes as pump sources for the first Tb^{3+}-based DPSSL [1]. The rapid development of blue-emitting diode lasers in the last decade culminated in simple and cost-efficient pump sources for visible lasers. In the recent experiments, an indium-gallium-nitride (InGaN)-based diode laser (iBeam Smart, Toptica Photonics) with an emission wavelength of 488.2 nm and a maximum output power of 200 mW served as the pump source. The sketch of the two mirror cavity utilizing a 28%Tb^{3+}:$LiLuF_4$ (Tb:LLF) as the active medium (Fig. 2) exposes the simplicity of the whole setup. Without any nonlinear conversion process, this system is even simpler than a green laser pointer, which requires an additional frequency conversion crystal.

Fig. 3 shows the laser results obtained at 544.1 nm in the green and at 587.4 nm in the yellow spectral region. The lasers exhibit high slope efficiencies of 52% and 22%, respectively, at transmissions of the output mirrors of 1.3% and 1.5%. In previous experiments [2] even higher efficiencies were observed at larger output coupling rates, however, at laser threshold values higher than the currently available diode pump power. At very low output coupling rates, the thresholds were found to be as low as 14 mW for the green and 27 mW for the yellow. The output power of both lasers is currently limited by the low power of the pump diode of only 200 mW, but power scaling by at least an order of magnitude is straightforward: watt-level multi-emitter cyan blue diodes are readily available and even further significant progress in these sources is foreseeable.

Further measurements performed at the ZLM indicate no quenching of the upper state lifetime even at much higher doping concentrations, which will allow the use of very small, highly doped gain elements enabling a miniaturization of these lasers. Previously, lasing was demonstrated even in TbF_3 with a Tb^{3+}-density of 2.2×10^{22} cm^{-3}, which is among the highest active ion densities of any laser crystal [3]. Future research in this direction will be facilitated by the recent establishment of a junior research group at the IKZ, which is focused on the development of fluoride crystals for laser applications.

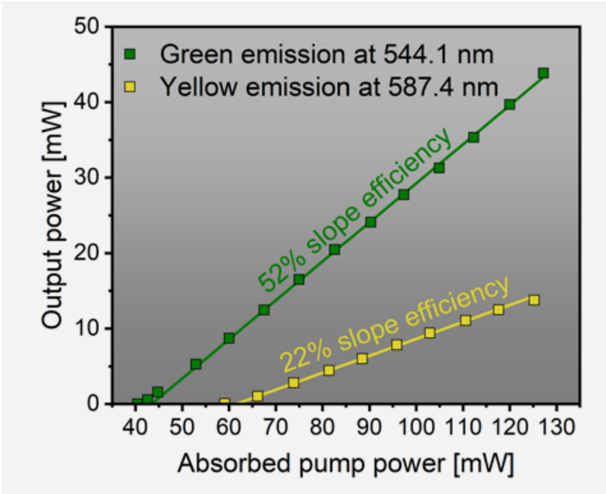


Fig. 3
Power curves of the Tb:LLF DPSSL emitting at green and the yellow wavelengths.

References

[1] E. Castellano-Hernández, S. Kalusniak, P. W. Metz, and C. Kränkel, *Diode-Pumped Laser Operation of Tb^{3+}:$LiLuF_4$ in the Green and Yellow Spectral Range,* Laser Photon. Rev. **14** (2), 1900229, (2020).

[2] E. Castellano-Hernández, P. W. Metz, M. Demesh, and C. Kränkel, *Efficient directly emitting high-power Tb^{3+}:$LiLuF_4$ laser operating at 587.5 nm in the yellow range,* Opt. Lett. **43** (19), 4791-4794, (2018).

[3] P. W. Metz, D.-T. Marzahl, A. Majid, C. Kränkel, and G. Huber, *Efficient continuous wave laser operation of Tb^{3+}-doped fluoride crystals in the green and yellow spectral regions,* Laser Photon. Rev. **10** (2), 335-344, (2016).

Progress in the development of aluminum nitride substrates for UV light-emitting diodes

T. Straubinger, C. Hartmann, U. Juda, J. Wollweber, K. Berger, L. Matiwe, A. Wagner, and M. Bickermann

Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Since September 2018, IKZ is leading a new joint project on the development of aluminum nitride substrates for light emitting and sensing diodes with short wavelength (230 nm) which is funded within the framework of the BMBF consortium "Advanced UV for Life" and coordinated by the IKZ.

IKZ and its partners will develop technology ready processes for the whole value-added chain starting from crystal gowth (IKZ), over crystal and surface preparation (Freiberger Compound Materials GmbH, Crystec GmbH) and growth of AlN buffer layers (Ferdinand Braun Institut, Leibniz Institut für Höchstfrequenztechnik, FBH) to the growth of optical active AlGaN layers and the fabrication of device structures (Technical University of Berlin, TUB). It is expected that the commercial availability of such UV devices will enable new applications in the fields of sensor technology (gases, biochemistry) and disinfection (water, medicine).

Meanwhile IKZ has demonstrated substrates with good bulk (DD < 10^4 cm^{-2}) and surface quality (no subsurface damage) as well as optimized substrate orientation (off-cut: 0.05° - 0.20°) to achieve epitaxial AlN buffer layers with dislocation densities (DD < 10^6 cm^{-2}) well below values achieved on sapphire substrates (DD > 10^8 cm^{-2}) which are up to now used as a standard substrate for UV devices.

Bulk aluminum nitride (AlN) is an alternative substrate for the production of Ultraviolet Light Emitting Diodes (UV LED) with short wavelengths near the theoretical limit of 210 nm. The advantage of these substrates is that, in contrast to the sapphire substrates typically used for UV LEDs, significantly fewer threading dislocations (TD) occur due to lattice mismatch and consequently there is less nonradiative recombination in the light emitting $Al_xGa_{1-x}N$ multi-quantum well layers resulting in higher light output [1].

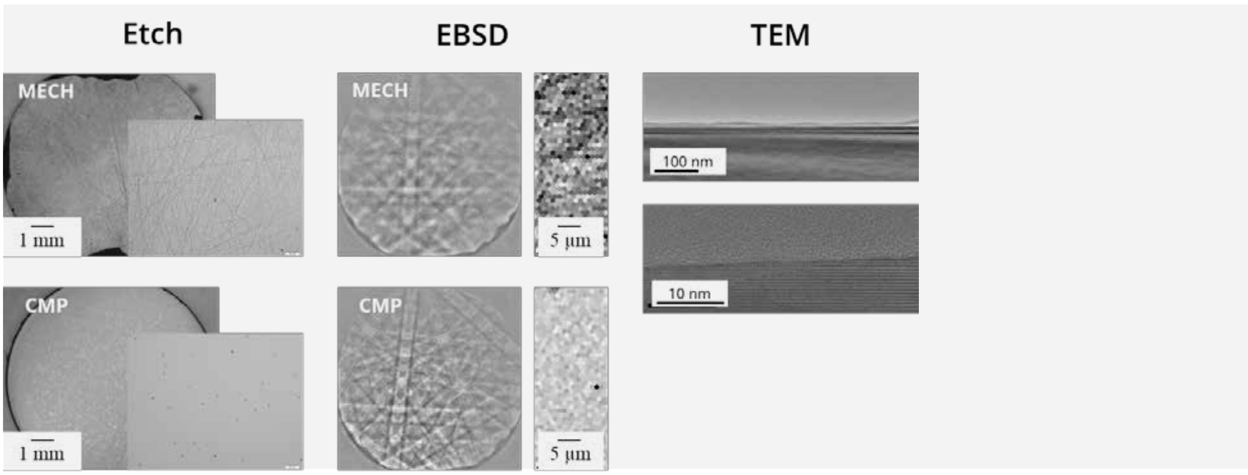


Fig. 1
Characterization of AlN substrate surfaces after different polishing levels.
Left: Etched AlN surfaces after mechanical polishing (top) showing scratch patterns and chemo mechanical polishing (bottom) showing no scratch pattern but etched dislocations.
Center: Kikuchi patterns and EBSD scan pictures (15 µm x 30 µm area) on AlN surfaces after mechanical polishing (top) showing local variations of the EBSD signal and a low average image quality factor (485) and chemo mechanical polishing (bottom) showing a homogeneous EBSD signal and a high average image quality factor (745).
Right: Transmission electron microscope image of AlN surface after chemo mechanical polishing. No dislocation lines on a 100 nm scale (top) and an undisturbed atomic structure are visible on a 10 nm scale (bottom).

Application Science

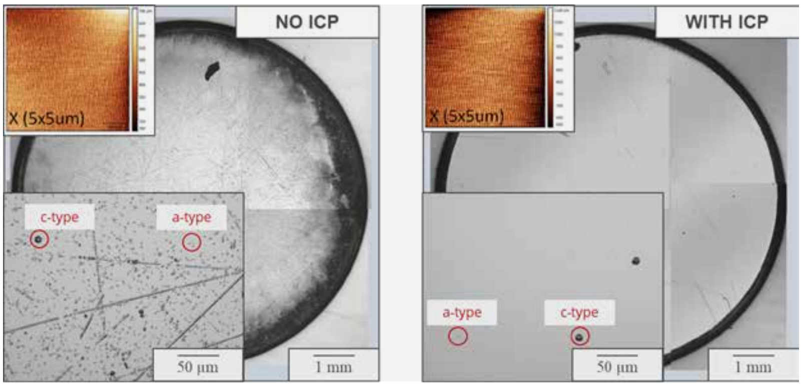


Fig. 2:
AlN substrates with MOVPE grown AlN-layer and subsequent defect etching with molten salts. The inserts show AFM-pictures with step-flow before defect etching. Left: No pre-treatment before MOVPE growth and resulting subsurface scratches revealed by defect etching and subsequent high dislocation density (DD > 10^8 cm^{-2}). Right: ICP etching pretreatment before MOVPE growth and resulting good surface quality and low dislocation density (DD < 10^6 cm^{-2}).

Main precondition for the growth of low defect AlN volume crystals is the use of seeds with high crystalline perfection and N-polar growth surfaces with high surface quality [2]. Additionally, the deposition of impurities on the growth surface must be avoided before the start of AlN growth. For this purpose, a sufficient thermal pre-cleaning of the source material ([O], [C] < 100 ppm) and a heating process prior to the actual growth process with a negative temperature difference between source and seed (T-K > T-Q) is essential [3]. Recent investigations at the IKZ [4] have also shown that low dislocation densities (DD < 10^4 cm^{-2}) can then be achieved at high growth temperatures and small temperature differences between source and seed surface during the actual growth phase.

Besides the substrate orientation, crystalline quality of the substrate surface is crucial for the quality of the AlN epitaxial layers grown with MOVPE. After sawing with an inner diameter or wire saw, the AlN wafers are first mechanically pre-polished and then chemo-mechanically end-polished on the Al side. In particular, damage to the crystalline structure close to the surface, which cannot usually be identified from the surface morphology, must be avoided. The high crystalline quality of AlN substrate surfaces produced with a polishing process developed and optimized at the IKZ could be verified with different characterization methods (Fig. 1).

A first polishing process variant developed on a laboratory scale at the IKZ was transferred to the industrial partner CrysTec at the beginning of 2019 and adapted to its existing production facilities. Although for all chemo mechanically polished surfaces neither before nor after epitaxy surface defects are visible in Normaski and AFM images, substrates which have been epitaxially overgrown without additional pre-treatment show linearly arranged clusters of dislocations which are presumably caused by surface near crystalline defects of the polished substrates (Fig. 2, left). These residual defects could be removed by an ICP etching process preceding the MOVPE growth and thus AlN layers without scratch like dislocation accumulations and low dislocation densities could be realized (Fig. 2, right).

This is considered as a breakthrough in the project, as from now on high quality AlN epitaxial layers on AlN substrates are available for the research on the optimization of optically active AlGaN layers and device structures. Anyway, in the medium term the surface quality will be further improved on the basis of the latest findings at the IKZ so that in future an ICP etching process prior to the epitaxy process will no longer be necessary.

Acknowledgements

The author would like to thank B. Weinert (Freiberger Compound Materials GmbH) and K. Peters (Crystec GmbH) for substrate preparation, A. Knauer (Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, FBH) for the growth of AlN-layers with MOVPE as well as T. Wernicke and M. Schilling (Technical University of Berlin, TUB) for AFM-measurements on AlN-layers.

The author also would like to thank IKZ colleagues T. Remmele and M. Albrecht for TEM-and EBSD-measurements.

References

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

[2] Z.G. Herro, D. Zhuang, R. Schlesser and Z. Sitar, J. Cryst. *Characterization of dislocation arrays in AlN single crystals grown by PVT,* Growth 312, 2519 (2010)

[3] R. Schlesser, V. Noveski and Z. Sitar, *Seeded growth process for preparing aluminium nitride single crystals,* WO Patent 2006110512

[4] C. Hartmann, L. Matiwe, J. Wollweber, I. Gamov, K. Irmscher, M. Bickermann and T. Straubinger, *Favourable growth conditions for the preparation of bulk AlN single crystals by PVT*, CrystEngComm 22, 1762 (2020)

Appendix

Publications

Publications

Abraham, R. J. S.; Shuman, V. B.; Portsel, L. M.; Lodygin, A. N.; Astrov, Y. A.; Abrosimov, N. V.; Paylov, S. G.; Hubers, H. W.; Simmons, S.; Thewalt, M. L. W., *Shallow donor complexes formed by pairing of double-donor magnesium with group-III acceptors in silicon.* Physical Review B; **99** (2019), 195207.

Agostini, M.; Bakalyarov, A. M.; Andreotti, E.; Balata, M.; Barabanov, I.; Baudis, L.; Barros, N.; Bauer, C.; Bellotti, E.; Belogurov, S.; Benato, G.; Bettini, A.; Bezrukov, L.; Bode, T.; Borowicz, D.; Brudanin, V.; Brugnera, R.; Budjas, D.; Caldwell, A.; Cattadori, C.; Chernogorov, A.; D'Andrea, V.; Demidova, E. V.; Di Marco, N.; Domula, A.; Doroshkevich, E.; Egorov, V.; Falkenstein, R.; Freund, K.; Gangapshev, A.; Garfagnini, A.; Gooch, C.; Grabmayr, P.; Gurentsov, V.; Gusev, K.; Hakenmuller, J.; Hegai, A.; Heisel, M.; Hemmer, S.; Hiller, R.; Hofmann, W.; Hult, M.; Inzhechik, L. V.; Csathy, J. J.; Jochum, J.; Junker, M.; Kazalov, V.; Kermaidic, Y.; Kihm, T.; Kirpichnikov, I. V.; Kirsch, A.; Kish, A.; Klimenko, A.; Kneissl, R.; Knopfle, K. T.; Kochetov, O.; Kornoukhov, V. N.; Kuzminov, V. V.; Laubenstein, M.; Lazzaro, A.; Lehnert, B.; Liao, Y.; Lindner, M.; Lippi, I.; Lubashevskiy, A.; Lubsandorzhiev, B.; Lutter, G.; Macolino, C.; Majorovits, B.; Maneschg, W.; Marissens, G.; Miloradovic, M.; Mingazheva, R.; Misiaszek, M.; Moseev, P.; Nemchenok, I.; Panas, K.; Pandola, L.; Pelczar, K.; Pullia, A.; Ransom, C.; Riboldi, S.; Rumyantseva, N.; Sada, C.; Salamida, F.; Salathe, M.; Schmitt, C.; Schneider, B.; Schonert, S.; Schutz, A. K.; Schulz, O.; Schwingenheuer, B.; Selivanenko, O.; Shevchik, E.; Shirchenko, M.; Simgen, H.; Smolnikov, A.; Stanco, L.; Vanhoefer, L.; Vasenko, A. A.; Veresnikova, A.; von Sturm, K.; Wagner, V.; Wegmann, A.; Wester, T.; Wiesinger, C.; Wojcik, M.; Yanovich, E.; Zhitnikov, I.; Zhukov, S. V.; Zinatulina, D.; Zsigmond, A. J.; Zuber, K.; Zuzel, G.; Collaboration, G., *Characterization of 30 Ge-76 enriched Broad Energy Ge detectors for GERDA Phase II.* European Physical Journal C; **79** (2019), 978.

Ahrling, R.; Boy, J.; Handwerg, M.; Chiatti, O.; Mitdank, R.; Wagner, G.; Galazka, Z.; Fischer, S. F., *Transport Properties and Finite Size Effects in beta-Ga_2O_3 Thin Films.* Scientific Reports; **9** (2019), 13149.

Althammer, M.; Singh, A. V.; Wimmer, T.; Galazka, Z.; Huebl, H.; Opel, M.; Gross, R.; Gupta, A., *Role of interface quality for the spin Hall magnetoresistance in nickel ferrite thin films with bulk-like magnetic properties.* Appl. Phys. Lett.; **115** (2019), 092403.

Anikeeva, M.; Albrecht, M.; Mahler, F.; Tomm, J. W.; Lymperakis, L.; Cheze, C.; Calarco, R.; Neugebauer, J.; Schulz, T., *Role of hole confinement in the recombination properties of InGaN quantum structures.* Scientific Reports; **9** (2019), 9047.

Beck, M.; Abrosimov, N. V.; Hubner, J.; Oestreich, M., *Impact of optically induced carriers on the spin relaxation of localized electron spins in isotopically enriched silicon.* Physical Review B; **99** (2019), 245201.

Bin Anooz, S.; Popp, A.; Gruneberg, R.; Wouters, C.; Schewski, R.; Schmidbauer, M.; Albrecht, M.; Fiedler, A.; Ramsteiner, M.; Klimm, D.; Irmscher, K.; Galazka, Z.; Wagner, G., *Indium incorporation in homoepitaxial beta-Ga_2O_3 thin films grown by metal organic vapor phase epitaxy.* J. Appl. Phys.; **125** (2019), 195702.

Boy, J.; Handwerg, M.; Ahrling, R.; Mitdank, R.; Wagner, G.; Galazka, Z.; Fischer, S. F., *Temperature dependence of the Seebeck coefficient of epitaxial beta-Ga_2O_3 thin films.* Apl Materials; **7** (2019), 022526.

Buchovska, I.; Dropka, N.; Kayser, S.; Kiessling, F. M., *The influence of travelling magnetic field on phosphorus distribution in n-type multi-crystalline silicon.* J. Cryst. Growth; **507** (2019), 299-306.

Lu-Chung, C., Maeda, K., Morito, H., Shiga, K., Miller, W., Fujiwara, K., *Effect of misorientation angle of grain boundary on the interaction with Σ3 boundary at crystal/melt interface of multicrystalline silicon.* MATERIALIA **7** (2019), 100357

DeAbreu, A., Bowness, C., Abraham, R.J.S., Medvedova, A., Morse, K., Riemann, H., Abrosimov, N., Becker, P., Pohl, H.-J., Thewalt, M., Simmons, S., *Characterization of the Si:Se+ Spin-Photon Interface.* Phys. Rev. Applied; **11** (2019), 44036

Demesh, M., Mudryi, A., Pavlyuk, A., Castellano-Hernández, E., Kränkel, C., Kuleshov, N., Cross sections and transition intensities of Tb^{3+} in $KY(WO_4)_2$. OSA Continuum, **2** (2019), 1378-1385

Dropka, N.; Holena, M.; Ecklebe, S.; Frank-Rotsch, C.; Winkler, J., *Fast forecasting of VGF crystal growth process by dynamic neural networks.* J. Cryst. Growth; **521** (2019), 9-14.

Dropka, N.; Ostrogorsky, A. G., *Interface control in vertical Bridgman growth by shaped and flat rotating baffles.* J. Cryst. Growth; **526** (2019), 125221.

Drozdowski, W.; Makowski, M.; Witkowski, M. E.; Wojtowicz, A. J.; Galazka, Z.; Irmscher, K.; Schewski, R., *beta-Ga_2O_3:Ce as a fast scintillator: An unclear role of cerium.* Radiation Measurements; **121** (2019), 49-53.

Publications

Drs, J.; Modsching, N.; Paradis, C.; Krankel, C.; Wittwer, V. J.; Razskazovskaya, O.; Sudmeyer, T., *Optical rectification of ultrafast Yb lasers: pushing power and bandwidth of terahertz generation in GaP.* Journal of the Optical Society of America B-Optical Physics; **36** (2019), 3039-3045.

Favaro, M.; Uecker, R.; Nappini, S.; Pis, I.; Magnano, E.; Bluhm, H.; van de Krol, R.; Starr, D. E., *Chemical, Structural, and Electronic Characterization of the (010) Surface of Single Crystalline Bismuth Vanadate.* Journal of Physical Chemistry C; **123** (2019), 8347-8359.

Feneberg, M.; Lidig, C.; White, M. E.; Tsai, M. Y.; Speck, J. S.; Bierwagen, O.; Galazka, Z.; Goldhahn, R., *Anisotropic optical properties of highly doped rutile SnO_2: Valence band contributions to the Burstein-Moss shift.* Apl Materials; **7** (2019), 022508.

Fiedler, A.; Galazka, Z.; Irmscher, K., *Electroluminescence of Cr3+ and pseudo-Stark effect in beta-Ga_2O_3 Schottky barrier diodes.* J. Appl. Phys.; **126** (2019), 213104.

Fiedler, A.; Schewski, R.; Galazka, Z.; Irmscher, K., *Static Dielectric Constant of beta- Ga_2O_3 Perpendicular to the Principal Planes (100), (010), and (001).* Ecs Journal of Solid State Science and Technology; **8** (2019), Q3083-Q3085.

Fujita, S.; Tanaka, H.; Kannari, F., *Intracavity second-harmonic pulse generation at 261 and 320 nm with a Pr^{3+}:YLF laser Q-switched by a Co^{2+}:$MgAl_2O_4$ spinel saturable absorber.* Opt. Express; **27** (2019), 38134-38146.

Galazka, Z.; Ganschow, S.; Schewski, R.; Irmscher, K.; Klimm, D.; Kwasniewski, A.; Pietsch, M.; Fiedler, A.; Schulze-Jonack, I.; Albrecht, M.; Schroder, T.; Bickermann, M., *Ultra-wide bandgap, conductive, high mobility, and high quality melt-grown bulk $ZnGa_2O_4$ single crystals.* Apl Materials; **7** (2019), 022512.

Gamov, I.; Hartmann, C.; Wollweber, J.; Dittmar, A.; Straubinger, T.; Bickermann, M.; Kogut, I.; Fritze, H.; Irmscher, K., *Carbon pair defects in aluminum nitride.* J. Appl. Phys.; **126** (2019), 215102.

Golz, C.; Galazka, Z.; Lahnemann, J.; Hortelano, V.; Hatami, F.; Masselink, W. T.; Bierwagen, O., *Electrical conductivity tensor of beta- Ga_2O_3 analyzed by van der Pauw measurements: Inherent anisotropy, off-diagonal element, and the impact of grain boundaries.* Physical Review Materials; **3** (2019), 124604.

Golz, C.; Galazka, Z.; Popp, A.; Bin Anooz, S.; Wagner, G.; Hatami, F.; Masselink, W. T., *Deep-level noise characterization of MOVPE-grown beta- Ga_2O_3.* Appl. Phys. Lett.; **115** (2019), 133504.

Grillo, A.; Barrat, J.; Galazka, Z.; Passacantando, M.; Giubileo, F.; Iemmo, L.; Luongo, G.; Urban, F.; Dubourdieu, C.; Di Bartolomeo, A., *High field-emission current density from - Ga_2O_3 nanopillars.* Appl. Phys. Lett.; **114** (2019), 193101.

Guguschev, C.; Klimm, D.; Brutzam, M.; Gesing, T. M.; Gogolin, M.; Paik, H.; Dittmar, A.; Fratello, V. J.; Schlom, D. G., *Single crystal growth and characterization of Ba2ScNbO6 - A novel substrate for $BaSnO_3$ films.* J. Cryst. Growth; **528** (2019), 125263.

Hagedorn, S.; Walde, S.; Mogilatenko, A.; Weyers, M.; Cancellara, L.; Albrecht, M.; Jaeger, D., *Stabilization of sputtered AlN/sapphire templates during high temperature annealing.* J. Cryst. Growth; **512** (2019), 142-146.

Hasse, K.; Huber, G.; Krankel, C., *Selective etching of fs-laser inscribed high aspect ratio microstructures in YAG.* Optical Materials Express; **9** (2019), 3627-3637.

Hidde, J.; Guguschev, C.; Klimm, D., *Thermal analysis and crystal growth of doped Nb_2O_5.* J. Cryst. Growth; **509** (2019), 60-65.

Hirsch, T.; Guguschev, C.; Kwasniewski, A.; Ganschow, S.; Klimm, D., *Investigation of the Nd2O3-Lu2O3-Sc2O3 phase diagram for the preparation of perovskite-type mixed crystals $NdLu_{1-x}Sc_xO_3$.* J. Cryst. Growth; **505** (2019), 38-43.

Hirschle, C.; Schreuer, J.; Ganschow, S.; Schulze-Jonack, I., *Thermoelastic properties of rare-earth scandates SmScO3, $TbScO_3$ and $DyScO_3$.* J. Appl. Phys.; **126** (2019), 165103.

Kamikawa, T.; Gandrothula, S.; Araki, M.; Li, H. J.; Oliva, V. B.; Wu, F.; Cohen, D.; Speck, J. S.; Denbaars, S. P.; Nakamura, S., *Realization of thin-film m-plane InGaN laser diode fabricated by epitaxial lateral overgrowth and mechanical separation from a reusable growth substrate.* Opt. Express; **27** (2019), 24717-24723.

Khirunenko, L.; Sosnin, M.; Duvanskii, A.; Abrosimov, N.; Riemann, H., *Features of the Formation of the BiBs Defect in Si.* Physica Status Solidi a-Applications and Materials Science; **216** (2019).

Kim, Y. M.; Markurt, T.; Kim, Y.; Zupancic, M.; Shin, J.; Albrecht, M.; Char, K., *Interface polarization model for a 2-dimensional electron gas at the $BaSnO_3$/$LaInO_3$ interface.* Scientific Reports; **9** (2019), 16202.

Publications

Kogut, I.; Hartmann, C.; Gamov, I.; Suhak, Y.; Schulz, M.; Schroder, S.; Wollweber, J.; Dittmar, A.; Irmscher, K.; Straubinger, T.; Bickermann, M.; Fritze, H., *Electromechanical losses in carbon- and oxygen-containing bulk AlN single crystals.* Solid State Ionics; **343** (2019), 115072.

Kowarik, S.; Bogula, L.; Boitano, S.; Carla, F.; Pithan, H.; Schafer, P.; Wilming, H.; Zykov, A.; Pithan, L., *A novel 3D printed radial collimator for x-ray diffraction.* Rev. Sci. Instrum.; **90** (2019), 035102.

Kriegner, D.; Springholz, G.; Richter, C.; Filet, N.; Muller, E.; Capron, M.; Berger, H.; Holy, V.; Dil, J. H.; Krempasky, J., *Ferroelectric Self-Poling in GeTe Films and Crystals.* Crystals; **9** (2019), 335.

Langenberg, E.; Saha, D.; Holtz, M. E.; Wang, J. J.; Bugallo, D.; Ferreiro-Vila, E.; Paik, H.; Hanke, I.; Ganschow, S.; Muller, D. A.; Chen, L. Q.; Catalan, G.; Domingo, N.; Malen, J.; Schlom, D. G.; Rivadulla, F., *Ferroelectric Domain Walls in $PbTiO_3$ Are Effective Regulators of Heat Flow at Room Temperature.* Nano Lett.; **19** (2019), 7901-7907.

Lee, W. C.; Wahila, M. J.; Mukherjee, S.; Singh, C. N.; Eustance, T.; Regoutz, A.; Paik, H.; Boschker, J. E.; Rodolakis, F.; Lee, T. L.; Schlom, D. G.; Piper, L. F. J., *Cooperative effects of strain and electron correlation in epitaxial VO_2 and NbO_2.* J. Appl. Phys.; **125** (2019), 082539.

Li, Z.; Krieft, J.; Singh, A. V.; Regmi, S.; Rastogi, A.; Srivastava, A.; Galazka, Z.; Mewes, T.; Gupta, A.; Kuschel, T., *Vectorial observation of the spin Seebeck effect in epitaxial $NiFe_2O_4$ thin films with various magnetic anisotropy contributions.* Appl. Phys. Lett.; **114** (2019), 232404.

Liddy, K. J.; Green, A. J.; Hendricks, N. S.; Heller, E. R.; Moser, N. A.; Leedy, K. D.; Popp, A.; Lindquist, M. T.; Tetlak, S. E.; Wagner, G.; Chabak, K. D.; Jessen, G. H., *Thin channel beta-Ga_2O_3 MOSFETs with self-aligned refractory metal gates.* Applied Physics Express; **12** (2019), 126501.

Makowski, M.; Drozdowski, W.; Witkowski, M. E.; Wojtowicz, A. J.; Irmscher, K.; Schewski, R.; Galazka, Z., *Tailoring the scintillation properties of beta-Ga_2O_3 by doping with Ce and codoping with Si.* Optical Materials Express; **9** (2019), 3738-3743.

Mazzolini, P.; Vogt, P.; Schewski, R.; Wouters, C.; Albrecht, M.; Bierwagen, O., *Faceting and metal-exchange catalysis in (010) beta-Ga_2O_3 thin films homoepitaxially grown by plasma-assisted molecular beam epitaxy.* Apl Materials; **7** (2019), 022511.

Medvedev, O.; Albrecht, M.; Vyvenko, O., *Asymmetry of the Atomic Core Structure of Dissociated a-Screw Dislocation in GaN Probed by Polarization Optical Spectroscopy.* Physica Status Solidi-Rapid Research Letters; **13** (2019), 1900169.

Medvedev, O.; Albrecht, M.; Vyvenko, O., *Unusual Polarization Dependence of Dislocation-Related Luminescence in n-GaN.* Physica Status Solidi a-Applications and Materials Science; **216** (2019).

Menzel, R.; Rost, H. J.; Kiesling, F. M.; Sylla, L., *Float-zone growth of silicon crystals using large-area seeding.* J. Cryst. Growth; **515** (2019), 32-36.

Modsching, N.; Drs, J.; Fischer, J.; Paradis, C.; Labaye, F.; Gaponenko, M.; Krankel, C.; Wittwer, V. J.; Sudmeyer, T., *Sub-100-fs Kerr lens mode-locked Yb:Lu_2O_3 thin-disk laser oscillator operating at 21 W average power.* Opt. Express; **27** (2019), 16111-16120.

Mogilatenko, A.; Knauer, A.; Zeimer, U.; Netzel, C.; Jeschke, J.; Unger, R. S.; Hartmann, C.; Wollweber, J.; Dittmar, A.; Juda, U.; Weyers, M.; Bickermann, M., *Crystal defect analysis in AlN layers grown by MOVPE on bulk AlN.* J. Cryst. Growth; **505** (2019), 69-73.

Mohamed, M.; May, M. M.; Kanis, M.; Brutzam, M.; Uecker, R.; van de Krol, R.; Janowitz, C.; Mulazzi, M., *The electronic structure and the formation of polarons in Mo-doped $BiVO_4$ measured by angle-resolved photoemission spectroscopy.* Rsc Advances; **9** (2019), 15606-15614.

Mulazzi, M.; Reichmann, F.; Becker, A.; Klesse, W. M.; Alippi, P.; Fiorentini, V.; Parisini, A.; Bosi, M.; Fornari, R., *The electronic structure of epsilon-Ga_2O_3.* Apl Materials; **7** (2019), 022522.

Nagata, T.; Bierwagen, O.; Galazka, Z.; Imura, M.; Ueda, S.; Yamashita, Y.; Chikyow, T., *Photoelectron spectroscopic study of electronic states and surface structure of an in situ cleaved In_2O_3 (111) single crystal.* Jpn. J. Appl. Phys.; **58** (2019), Sddg06.

Nagata, T.; Bierwagen, O.; Galazka, Z.; Ueda, S.; Imura, M.; Yamashita, Y.; Chikyow, T., *Photoelectron spectroscopic study on electronic state and electrical properties of SnO_2 single crystals.* Jpn. J. Appl. Phys.; **58** (2019), 080903.

Nentwich, M.; Weigel, T.; Zschornak, M.; Richter, C.; Kohler, T.; Mehner, E.; Novikov, D.; Meyer, D. C., *$LiTaO_3$ defect structures by means of forbidden reflections.* Acta Crystallographica a-Foundation and Advances; **75** (2019), E289-E289.

Publications

Pavlov, S. G.; Abrosimov, N. V.; Shuman, V. B.; Portsel, L. M.; Lodygin, A. N.; Astrov, Y. A.; Zhukavin, R. K.; Shastin, V. N.; Irmscher, K.; Pohl, A.; Hubers, H. W., *Even-Parity Excited States in Infrared Emission, Absorption, and Raman Scattering Spectra of Shallow Donor Centers in Silicon.* Physica Status Solidi B-Basic Solid State Physics; **256** (2019), 1800514.

Pejchal, J.; Guguschev, C.; Schulze, M.; Jary, V.; Mihokova, E.; Rubesova, K.; Jakes, V.; Barta, J.; Nikl, M., *Luminescence and scintillation properties of strontium hafnate and strontium zirconate single crystals.* Opt. Mater.; **98** (2019), 109494.

Plate, M.; Dadzis, K.; Krauze, A.; Menzel, R.; Virbulis, J., *Validation of a 3D mathematical model for feed rod melting during floating zone Si crystal growth.* J. Cryst. Growth; **521** (2019), 46-49.

Powderly, K. M.; Guo, S.; Stolze, K.; Carnicom, E. M.; Cava, R. J., *Synthesis and characterization of the novel antiferromagnet $LaNiB_3O_7$.* J. Solid State Chem.; **272** (2019), 113-117.

Qi, X. F.; Liu, L. J.; Riberi-Beridot, T.; Mangelinck-Noel, N.; Miller, W., *Simulation of grain evolution in solidification of silicon on meso-scopic scale.* Computational Materials Science; **159** (2019), 432-439.

Rovaris, F.; Zoellner, M. H.; Zaumseil, P.; Marzegalli, A.; Di Gaspare, L.; De Seta, M.; Schroeder, T.; Storck, P.; Schwalb, G.; Capellini, G.; Montalenti, F., *Dynamics of crosshatch patterns in heteroepitaxy.* Physical Review B; **100** (2019), 085307.

Sander, M.; Bauer, R.; Kabanova, V.; Levantino, M.; Wulff, M.; Pfuetzenreuter, D.; Schwarzkopf, J.; Gaal, P., *Demonstration of a picosecond Bragg switch for hard X-rays in a synchrotron-based pump-probe experiment.* Journal of Synchrotron Radiation; **26** (2019), 1253-1259.

Schewski, R.; Lion, K.; Fiedler, A.; Wouters, C.; Popp, A.; Levchenko, S. V.; Schulz, T.; Schmidbauer, M.; Bin Anooz, S.; Gruneberg, R.; Galazka, Z.; Wagner, G.; Irmscher, K.; Scheffler, M.; Draxl, C.; Albrecht, M., *Step-flow growth in homoepitaxy of beta-Ga_2O_3 (100)-The influence of the miscut direction and faceting.* Apl Materials; **7** (2019), 022515.

Schubert, M.; Mock, A.; Korlacki, R.; Knight, S.; Galazka, Z.; Wagner, G.; Wheeler, V.; Tadjer, M.; Goto, K.; Darakchieva, V., *Longitudinal phonon plasmon mode coupling in beta-Ga_2O_3.* Appl. Phys. Lett.; **114** (2019), 102102.

Sennikov, P. G.; Kornev, R. A.; Abrosimov, N. V.; Bulanov, A. D.; Gavva, V. A.; Potapov, A. M., *Feasibility study of the production of bulk stable Ge isotopes by the hydrogen plasma chemical reduction of fluorides.* Materials Science and Engineering B-Advanced Functional Solid-State Materials; **244** (2019), 1-5.

Shastin, V. N.; Zhukavin, R. K.; Kovalevsky, K. A.; Tsyplenkov, V. V.; Rumyantsev, V. V.; Shengurov, D. V.; Pavlov, S. G.; Shuman, V. B.; Portsel, L. M.; Lodygin, A. N.; Astrov, Y. A.; Abrosimov, N. V.; Klopf, J. M.; Hubers, H. W., *Chemical Shift and Exchange Interaction Energy of the 1s States of Magnesium Donors in Silicon. The Possibility of Stimulated Emission.* Semiconductors; **53** (2019), 1234-1237.

Shuman, V. B.; Lodygin, A. N.; Portsel, L. M.; Yakovleva, A. A.; Abrosimov, N. V.; Astrov, Y. A., *Decomposition of a Solid Solution of Interstitial Magnesium in Silicon.* Semiconductors; **53** (2019), 296-297.

Siekacz, M.; Wolny, P.; Ernst, T.; Grzanka, E.; Staszczak, G.; Suski, T.; Feduniewicz-Zmuda, A.; Sawicka, M.; Moneta, J.; Anikeeva, M.; Schulz, T.; Albrecht, M.; Skierbiszewski, C., *Impact of the substrate lattice constant on the emission properties of InGaN/GaN short-period superlattices grown by plasma assisted MBE.* Superlattices Microstruct.; **133** (2019), 106209.

Stanchu, H. V.; Kuchuk, A. V.; Mazur, Y. I.; Li, C.; Lytvyn, P. M.; Schmidbauer, M.; Maidaniuk, Y.; Benamara, M.; Ware, M. E.; Wang, Z. M. M.; Salamo, G. J., *Local Strain and Crystalline Defects in GaN/AlGaN/GaN(0001) Heterostructures Induced by Compositionally Graded AlGaN Buried Layers.* Crystal Growth & Design; **19** (2019), 200-210.

Tetzner, K.; Treidel, E. B.; Hilt, O.; Popp, A.; Bin Anooz, S.; Wagner, G.; Thies, A.; Ickert, K.; Gargouri, H.; Wurfl, J., *Lateral 1.8 kV beta-Ga_2O_3 MOSFET With 155 MW/cm^2 Power Figure of Merit.* Ieee Electron Device Letters; **40** (2019), 1503-1506.

Thieme, N.; Keil, M.; Meier, D.; Bonisch, P.; Dadzis, K.; Patzold, O.; Stelter, M.; Buttner, L.; Czarske, J., *Directional solidification of gallium under time-dependent magnetic fields with in situ measurements of the melt flow and the solid-liquid interface.* J. Cryst. Growth; **522** (2019), 221-229.

Toncelli, A.; Xu, J. H.; Tredicucci, A.; Heuer, A. M.; Krankel, C., *Mid-Infrared spectroscopic characterization of Pr^{3+}:Lu_2O_3.* Optical Materials Express; **9** (2019), 4464-4473.

Publications

Treekamol, Y.; Schieda, M.; Herrmann-Geppert, I.; Klassen, T., *Optimized photoactive coatings prepared with functionalized TiO_2.* Int. J. Hydrogen Energy; **44** (2019), 31800-31807.

Vazquez-Cordova, S. A.; Aravazhi, S.; Heuer, A. M.; Krankel, C.; Yong, M. S.; Garcia-Blanco, S. M.; Herek, J. L.; Pollnau, M., *Energy-transfer upconversion and excited-state absorption in $KGd_xLu_yEr_{1-x-y}(WO_4)_2$ waveguide amplifiers.* Optical Materials Express; **9** (2019), 4782-4795.

von Helden, L.; Bogula, L.; Janolin, P. E.; Hanke, M.; Breuer, T.; Schmidbauer, M.; Ganschow, S.; Schwarzkopf, J., *Huge impact of compressive strain on phase transition temperatures in epitaxial ferroelectric $K_xNa_{1-x}NbO_3$ thin films.* Appl. Phys. Lett.; **114** (2019), 232905.

Wahila, M. J.; Paez, G.; Singh, C. N.; Regoutz, A.; Sallis, S.; Zuba, M. J.; Rana, J.; Tellekamp, M. B.; Boschker, J. E.; Markurt, T.; Swallow, J. E. N.; Jones, L. A. H.; Veal, T. D.; Yang, W. L.; Lee, T. L.; Rodolakis, F.; Sadowski, J. T.; Prendergast, D.; Lee, W. C.; Doolittle, W. A.; Piper, L. F. J., *Evidence of a second-order Peierls-driven metal-insulator transition in crystalline NbO_2.* Physical Review Materials; **3** (2019), 074602.

Wang, J. Y.; Lin, F. R.; Verzhbitskiy, I.; Watanabe, K.; Taniguchi, T.; Martin, J.; Eda, G., *Polarity Tunable Trionic Electroluminescence in Monolayer WSe_2.* Nano Lett.; **19** (2019), 7470-7475.

Weinstein, O.; Virozub, A.; Miller, W.; Brandon, S., *Modeling anisotropic shape evolution during Czochralski growth of oxide single crystals.* J. Cryst. Growth; **509** (2019), 71-86.

Wienold, M.; Pavlov, S. G.; Abrosimov, N. V.; Hubers, H. W., *High-resolution, background-free spectroscopy of shallow-impurity transitions in semiconductors with a terahertz photomixer source.* Appl. Phys. Lett.; **114** (2019), 092103.

Wolff, N.; Klimm, D.; Ganschow, S.; Siche, D., *Thermodynamic Investigation of Ternary Delafossite Crystals.* Cryst. Res. Technol.; **54** (2019), 1900036.

Wouters, C., Markurt, T., Bierwagen, O., Sutton, C., Albrecht, M., *In situ Transmission Electron Microscopy Annealing for Crystallization and Phase Stability Studies in the Ga2O3-In2O3 System*. Microscopy and Microanalysis, **25** (2019), 1890-1891

Wouters, C.; Markurt, T.; Albrecht, M.; Rotunno, E.; Grillo, V., *Influence of 2s Bloch wave state excitations on quantitative HAADF STEM imaging.* Physical Review B; **100** (2019), 184106.

Yarykin, N.; Shuman, V. B.; Portsel, L. M.; Lodygin, A. N.; Astrov, Y. A.; Abrosimov, N. V.; Weber, J., *DLTS Investigation of the Energy Spectrum of Si:Mg Crystals.* Semiconductors; **53** (2019), 789-794.

Zhukavin, R. Z., Kovalevskii, K. A., Choporova, Y.Y., Tsyplenkov, V. V., Gerasimov, V. V., Bushuikin, P. A., Knyazev, B. A., Abrosimov, N. V., Pavlov, S. G., Hübers, H.-W., Shastin, V. N., *Relaxation Times and Population Inversion of Excited Statesof Arsenic Donors in Germanium.* JEPT Letters; **110** (2019), 677-682

Zhukavin, R. K., Pavlov, S.G., Pohl, A., Abrosimov, N.V., Riemann, H., Redlich, B., Hübers, H.-W., Shastin, V. N., *Stimulated Terahertz Emission of Bismuth Donors in Uniaxially Strained Silicon under Optical Intracenter Excitation*. Semiconductors; **53** (2019), 1255-1257

Zoellner, M. H.; Chahine, G. A.; Lahourcade, L.; Mounir, C.; Manganelli, C. L.; Schulli, T. U.; Schwarz, U. T.; Zeisel, R.; Schroeder, T., *Correlation of Optical, Structural, and Compositional Properties with V-Pit Distribution in InGaN/GaN Multiquantum Wells.* Acs Applied Materials & Interfaces; **11** (2019), 22834-22839.

Talks and Posters

Talks and Posters

Invited talks at national and international conferences

N. Abrosimov, M. Czupalla, N. Dropka, J. Fischer, K.-P. Gradwohl, O. Gybin, K. Irmscher, J. Janicsko-Csathy, U. Juda, S. Kayser, F.M. Kießling, W. Miller, M. Pietsch, R. Sumathi, *High Purity Germanium project at IKZ*, 4th PIRE Collaboration Meeting, München, Germany, 2019

M. Albrecht, R. Schewski, C. Wouters, K. Irmscher, A. Fiedler, M. Schmidbauer, A. Popp, Z.Galazka, G. Wagner, P. Mazzolini, P.Vogt and O. Bierwagen, K. Lion, C. Draxl, S. Levchenko, M. Scheffler, *Growth mode and surface orientation in the homoepitaxial growth of β-Ga_2O_3: the influence of the miscut direction and faceting*, Photonics West, San Francisco, USA, 2019

M. Albrecht, T. Schulz, Lymperakis, M. Siekacz, J. Moneta, M. Anikeeva, C. Freysoldt, J.Smalc-Koziorowska, Z. Chen, X. Zheng, B. Shen, C. Chèze, C.Skierbiszewski, X. Q. Wang, Neugebauer, *Challenges in shifting the emission of InGaN quantum wells towards the red*, International Conference on Nitride Semicondcuctors 13, Seattle, USA, 2019

M. Albrecht, R. Schewski, A. Fielder, M. Baldini, S. Bin Anooz, G. Wagner, Z.Galazka, K. Irmscher, A. Popp, K. Lion, and C. Draxl, *Ga_2O_3 from Materials to Devices,* International Conference on Silicon Carbide and Related Materials 2019, Kyoto, Japan, 2019

I. Buchovska, N. Dropka, F.-M. Kiessling, *Adjustment of resistivity for phosphorus doped n-type multicrystalline silicon*, GPCCG-3, Poznań, Polen, 2019

N. Dropka, M. Holena, S. Ecklebe, Ch. Frank-Rotsch, J. Winkler, *Artificial intelligence in crystal growth,* ICCGE-19 / OMVPE-19 / ISSCG-17, Keystone, USA, 2019

N. Dropka, M. Holena, S. Ecklebe, Ch. Frank-Rotsch, J. Winkler, *Artificial intelligence in crystal growth,* Siltronic meeting, Burghausen, Germany, 2019

O. Ernst, F. Lange, K. Eylers, J. Bonse, J. Krüger, T. Boeck, *Reorganization of thin metal layers by (de) wetting phenomena for microelectronic applications*, WE-Heraeus-Seminar: Wetting on Soft or Micro-structured Surfaces, Bad Honnef, Germany, 2019

P. Gaal, *Strain-induced dynamics monitored by time-resolved x-ray diffraction*, Workshop on Short Pulse Science with the Extremely Brilliant Source, Grenoble, France, 2019

Z. Galazka, *Transparent Semiconducting Oxides – Bulk Single Crystals and Basic Properties*, The 11th International Conference on the Science and Technology for Advanced Ceramics, Tsukuba, Japan, 2019

Z. Galazka, *Czochralski-grown bulk β-Ga_2O_3 single crystals doped with mono-, di-, tri-, and tetravalent ions, and VGF-grown bulk ZnGa2O4 single crystals*, IWGO-3, Columbus, USA, 2019

S. Ganschow, C. Guguschev, I. Schulze-Jonack, D. Klimm, L. von Helden, L. Bogula, M. Schmidbauer, J. Schwarzkopf, *Growth of rare-earth scandate single crystals as substrates for epitaxial films*, EUROMAT 2019, Stockholm, Sweden, 2019

C. Guguschev, D. Klimm, M. Brützam, T. M. Gesing, M. Gogolin, J. Hidde, T. Markurt, S. Ganschow, J. Schwarzkopf, M. Bickermann, D. G. Schlom, *Growth and characterization of large-lattice-parameter perovskite substrate single crystals for ferroelectric films and devices,* ICCGE-19 / OMVPE-19, Keystone, Colorado, USA, 2019

C. Guguschev, S. Ganschow, D. Klimm, M. Brützam, I. Schulze-Jonack, M. Bickermann, *27 years of progress in perovskite-type substrate crystal growth at the IKZ,* ICCGE-19 / OMVPE-19, Keystone, Colorado, USA, 2019

C. Guguschev, J. Pejchal, M. Schulze, A. Uvarova, T. Schwaigert, D. Klimm, S. Ganschow, M. Bickermann, *Exploring the advantages of the optical floating zone technique on the growth of high melting point perovskites and other oxides,* 3rd workshop Floating Zone Technique, Oxford, UK, 2019

D. Klimm, *Thermal Analysis and Thermodynamic Calculations in Rare-Earth Oxide Based Systems,* FactSage User Meeting, Herzogenrath, Germany, 2019

C. Kränkel, *Short course: Emerging solid-state gain media,* Advanced Solid-State Lasers Conference 2019, Vienna, Austria, 2019

J. Martin, *New perspectives for 2D-Layer Transfer,* CETC, 46 Workshop on Crystalline Materials, Tiajing, China, 2019

Talks and Posters

R. Menzel, *Numerical simulation of the float zone process for silicon: Comparison of modeling approaches in COMSOL Multiphysics,* International Symposium on Modeling of Crystal Growth Processes and Devices, Chennai, India, 2019

R. Menzel, *Modelling of the FZ Growth of Silicon Single Crystals with Large Diameter*, CETC, 46 Workshop on Crystalline Materials, Tiajing, China, 2019

A. Popp, *Homoepitaxial growth if semiconducting β-Ga_2O_3 film by MOVPE*, CETC, 46 Workshop on Crystalline Materials, Tiajing, China, 2019

A. Popp, S. Anooz, G. Wagner, A. Fiedler, R. Schewski, K. Irmscher, Z. Galazka, M. Albrecht, *correlation between substrate miscut angle and growth rate for homoepitaxial β-Ga_2O_3 layers grown by MOVPE,* IWGO 19, Ohio, USA, 2019

R. Radhakrishnan Sumathi, J. Janicskó- Csathy, K.P. Gradwohl, O. Gybin, N. Abrosimov, *High purity germanium crystals for detector application – the path traveled so far and the way ahead*, nanoGe Fall meeting 2019, Berlin, Germany, 2019

R. Radhakrishnan Sumathi, G*ermanium as an emerging strategic material for next-generation devices and applications*, Semicon-Europe 2019, München, Germany, 2019

D. Rettenwander, J. Ring, S. Smetaczek, S. Ganschow, S. Berendts, A. Limbeck, *Incestigating H+/Li+ exchange in cubic LLZO ganets: Spatially resolved H-determination unsing LIBS*, 2nd world conference on solid electrolytes for advanced applications: Garnets and competitors, Japan, 2019

D. Rettenwander, S. Smetaczek, J. Ring, E. Pycha, S. Ganschow, S. Berendts, A. Limbeck, J. Fleig, *Field stress experiments on cubic LLZO garnets: Investigation of the electrochemical stability*, 2nd world conference on solid electrolytes for advanced applications: Garnets and competitors Japan, 2019

T. Schröder, V. J. Fratello , M. Bickermann, D.G. Schlom, *Challenges and Opportunities for Innovative Crystal-line Materials in Europe – an IKZ perspective*, GPCCG 3, Poznan, Poland, 2019

T. Schröder, *Modern Growth, Characterization & Appli-cations of SiGe Volume Crystals & Thin Films*, ISCSI-VIII, Sendai, Japan, 2019

T. Schröder, *Crystalline Materials as technology enablers in electronics & photonics*, CETC Workshop, School of Electronics, Tianjin, China, 2019

T. Schröder, *On the role crystals an key enabling materials for disruptive technologies,* CETC, 46 Workshop on Crystalline Materials, Tiajing, China, 2019

Invited seminars at national and international institutions

N.V. Abrosimov, *Avogadro project and 28Si story*, Seminar in honour of Michael Thewalt, Simon Fraser University, Burnaby, Canada, 2019

N.V. Abrosimov, *Growth of 28Si crystals for preparation of Si spheres,* PTB Seminar, Braunschweig, Germany, 2019

P. Gaal, *Deformation dynamics in thin films and nano-structures*, Leibniz-Institut für Festkörperforschung, Institut für Metallische Werkstoffe, Berlin, Germany, 2019

K. Irmscher, *Gallium oxide from materials to devices*, Physikalisches Kolloquium, TU BA Freiberg, Germany, 2019

D. Klimm, *Thermodynamics of Crystal Growth,* International Summer School on Crystal Growth (ISSCG-17), Colorado, USA, 2019

C. Kränkel, *Progress and applications of ultrafast lasers based on rare-earth doped sesquioxides*, Colloquium at the National Key Laboratory of Laser & Infrared Systems, Ministry of Education, Qingdao, China, 2019

C. Kränkel, *Growth and laser operation of rare-earth doped sesquioxides*, Colloquium at the School of Information Science and Engineering and Shandong Provincial Key Laboratory of Laser technology and Application, Shandong University, Jinan, China, 2019

C. Kränkel, *Continuous wave and pulsed visible lasers based on Pr- and Tb-doped fluoride crystals*, Colloquium at the National Key Laboratory of Laser & Infrared Systems, Ministry of Education, Qingdao, China, 2019

Talks and Posters

C. Kränkel, *Absorptionsspektroskopie an Seltenerd-dotierten Laserkristallen*, PerkinElmer UV-Vis/NIR Seminar, Rodgau, Germany, 2019

J. Martin, *New perspectives for 2D-Layer Transfer,* IOP CAS - IRIS HU Workshop, Dongguan, Beijing, China, 2019

J. Martin, *Technologies for novel hetero-structures: alternative growth methods and layer transfer*, PDI Institute Seminar, Berlin, Germany, 2019

R. Schewski, K. Lion, A. Fiedler, C. Wouters, A. Popp, S. V. Levchenko, T. Schulz, M. Schmidbauer, S. Bin Anooz, R. Grüneberg, *Fundamental insights into growth and characterisation of homoepitaxial b-Ga_2O_3 layer for electronic applicatio,* Seminar Talk Torun, Poland, 2019

T. Schröder, *IKZ´s innovations in & by crystalline materials: The example of Ga_2O_3*, ABB Research Center, Zürich, Switzerland, 2019

T. Schröder, *IKZ´s future R & D strategy: From science & technology to service & transfer*, Kistler AG Research Center, Zürich, Switzerland, 2019

T. Schröder, *To control materials means to control technologies – on the need of high performing crystalline materials,* The 46th Research Institute of China Electronics Technology Group Corporation (CETC), Tianjin, China, 2019

T. Schröder, *Key technology enablers: Crystalline Materials in Electronics & Photonics,* Kolloquium Forschungszentrum Jülich, Germany 2019

T. Schröder, *IKZ – The European Flagship R & D Center for Innovations in and by Crystalline Materials*, OXIDE Corporation, Kofu, Japan, 2019

T. Schröder, *Crystalline Materials as technology enablers in electronics & photonics*, Jiantong University, School of Electronics, Xi'an, China, 2019

T. Schröder, *Innovative kristalline Materialien für Grundlagenforschung & Zukunftstechnologien,* Adlershofer Forschungsforum 2019, IGAFA Berlin-Adlershof, Germany, 2019

T. Schröder, *Examples on Innovative Crystalline Materials & Novel Materials Science Method*, Physikalisches Kolloquium, Otto von Guericke Universität Magdeburg, Magdeburg, Germany, 2019

Oral contributions at national and international conferences, workshops or seminars

N. Abrosimov, M. Czupalla, N. J. Fischer, R. Sumathi, *Czochralski growth of Phosphorus and Boron doped Germanium*, GPCCG-3 Poznań, Polen, 2019

M. Bickermann, Z. Galazka, I. Hanke, S. Ganschow, R. Uecker, D. Klimm, A. Popp, *Crystals and Substrates for Semiconducting Oxide Applications,* DGKK-Arbeitskreis Massive Halbleiter, Berlin, Germany, 2019

M. Bickermann, *Jan Czochralski and the decisive impact of his invention on modern technology*, Czochralski-Milestone-Event der IEEE, htw- Berlin, Berlin, Germany, 2019

M. Bickermann, *Native AlN Substrates*, 1. Internationalen Workshop über AlGaN-basierte UV-Laserdioden (IWUVLD-2019), Berlin, Gemany, 2019

S. Bin Anooz, G. Wagner, R. Grüneberg, A. Fiedler, K. Irmscher, R. Schweski, M. Albrecht, Z. Galazka, A. Popp, *Optimization of β-Ga_2O_3 film growth on miscut (100) β-Ga_2O_3 subtrates by MOVPE,* Transparent Conductive Oxides – Fundamentals and Applications (TCO2019), Leipzig, Germany, 2019

K. Böttcher, W. Miller, S. Ganschow, *Numerical Modelling of the Czochralski growth of $NdScO_3$ single crystals,* DGKK-Arbeitskreis Massive Halbleiter, Berlin, Germany, 2019

I. Buchovska, N. Dropka, K. Dadzis, F.-M. Kiessling, *Homogenization of resistivity for n-type multicrystaline silicon,* DGKK-Arbeitskreis Massive Halbleiter, Berlin, Germany, 2019

E. Castellano-Hernandez, C. Kränkel, *Diode-pumped Tb^{3+}-doped laser with direct emission in the visible range*, DPG-Frühjahrstagung, München, Deutschland, 2019

E. Castellano-Hernández, S. Kalusniak, and C. Kränkel, *Diode-pumped yellow laser emission of Tb^{3+}:$LiLuF_4$*, Advanced Solid State Lasers Conference (ASSL) Vienna, Austria, 2019

E. Castellano-Hernandez, C. Kränkel, *Diode-pumped visible laser operation of Tb^{3+}:$LiLuF_4$*, CLEO/Europe-EQEC Conference, Munich, Germany, 2019

Talks and Posters

K. Dadzis, I. Buchovska, F.-M. Kiessling, *3D numerical simulation of melt flow and dopant transport in directional solidification of silicon*, DGKK-Arbeitskreis Massive Halbleiter, Berlin, Germany, 2019

K. Dadzis, K. Dadzis, U. Juda, M. Albrecht, R. Menzel, C. Reimann, C. Kranert, R. Weingärtner, M. Müller, M. Ehrl, *Caracterization of silicon crystals grown from melt in a granulate crucible*, 18th Conference on Defects-Recognition, Imaging and Physics in Semiconductors (DRIP XVIII), Berlin, Germany, 2019

N. Dropka, A. Ostrogorsky, *Enhanced Czochralski crystal growth with submerged rotating baffle,* BIFD 2019, Limerick, Ireland, 2019

J. Drs, N. Modsching, C. Paradis, C. Kränkel, V. J. Wittwer, O. Razskazovskaya, *High-power 0.33 mW broadband THz source driven by an ultrafast Yb-based thin-disk laser oscillator*, Conference on Lasers and Electro-Optics (CLEO/Europe-EQEC) 2019, Munich, Germany, 2019

S. Ecklebe, J. Winkler, C. Frank-Rotsch, N. Dropka, *Towards model predictive control for VGF growth using artificial neural networks*, ICCGE-19 / OMVPE-19 / ISSCG-17, Keystone, USA, 2019
O. Ernst, K. Eylers, F. Lange, J. Bonse, J. Krüger, T. Boeck, *Manufacturing of local defined nano- and microstructures for semiconductor devices by dewetting phenomena*, 45th international conference on micro & nano engineering, Rhodes, Greece, 2019

A. Fiedler, A. Popp, S. Anooz, G. Wagner, Z. Galazka, R. Schewski, M. Albrecht, K. Irmscher, *Comparison of the electrical properties of β-Ga_2O_3 layers homoepitaxially grown by MOVPE and HVPE,* IWGO 19, Ohio, USA, 2019

P. Fielitz, S. Ganschow, K. Kelm, G. Borchardt, *Impact of titanium doping on Al self-diffusion in alumina*, Diffusion Fundamentals 8, Erlangen, Germany, 2019

I. Gamov, K. Irmscher, E. Richter, M. Meyers, *Identification of Tri-Carbon Defects in Gallium* Nitride DRIP XVIII, Berlin, Germany, 2019

I. Gamov, K. Irmscher, E. Richter, M. Meyers, *Identification of Tri-Carbon Defects in Gallium Nitride* DGKK-Arbeitskreis Massive Halbleiter, Berlin, Germany, 2019

K.-P. Gradwohl, O. Gybin, J. Janicsko-Csathy, U. Juda, N. Abrosimov, F.-M. Kießling, R. Radhakrisnan Sumathi, *Investigation of dislocation networks in high-purity germanium for detector applications,* GPCG-3, Poznań, Polen, 2019

K.-P. Gradwohl, O. Gybin, J. Janisko-Csathy, U. Juda, M. Schidbauer, R. Radhakrishnan Sumathi, *Vacancy clustering in dislocation-free high-purity germanium*, DRIP XVIII, Berlin, Germany, 2019

K.-P. Gradwohl, A. Gybin, J. Janicsko-Csathy, A. Danilewsky, M. Roder, M. Schmidbauer, R. Radhakrishnan Sumathi, *Growth and Investigation of dislocation-free HPGe crystals*, DGKK-Arbeitskreis Massive Halbleiter, Berlin, Germany, 2019

C. Guguschev, D. Klimm, M. Brützam, T. M. Gesing, M. Gogolin, H. Paik, Z. Chen, T. Markurt, A. Kwasniewski, A. Dittmar, D.A. Muller, V. J. Fratello, M. Bickermann, D.G. Schlom, *Single crystal growth and characterization of $La_{1-x}Nd_xSc_{1-y}Lu_yO_3$ and Ba_2ScNbO_6 - lattice-matched substrates for $BaSnO_3$ films and devices,* 26th IWOE- International Workshop on Oxide Electronics, Kyoto, Japan, 2019

C. Hiebl, D. Young, M. Gombotz, R. Wagner, S. Ganschow, M. Meven, G.J. Redhammer, H.M.R. Wilkening, D. Rettenwander, *The impact of humidity and aqueous solutions on the structural and ion dynamical properties of cubic $Li_7La_3Zr_2O_{12}$ garnets studied on single crystals*, Joint ISAF-ICE-EMF-IWPM-PFM meeting 2019, Lausanne, Switzerland, 2019
C. Hirschle, S. Ganschow, J. Schreuer, I. Schulze-Jonack, *Elastic instabilities if rare-earth scandates $SmScO_3$, $TbScO_3$ and $DyScO_3$*, GEO Münster und MRS Fall Meeting, Münster, Germany, 2019

C. Hirschle, S. Ganschow, J. Schreuer, I. Schulze-Jonack, *Thermoelastic properties of rare-earth scandates $SmScO_3$, $TbScO_3$ and $DyScO_3$,* GEO Münster und MRS Fall Meeting, Münster, Germany, 2019

K. Hasse, C. Kränkel, *Yb:CALGO waveguide laser written with 1 MHz-repetition rate fs-laser*, Advanced Solid-State Lasers Conference 2019, Vienna, Austria, 2019

L. von Helden, L. Bogula, P.-E. Janolin, M. Hanke, S. Liang, T. Breuer, R. Wördenweber, M. Schmidbauer, S. Ganschow, and J. Schwarzkopf, *Huge impact of compressive strain on phase transition temperatures in epitaxial, ferroelectric KNN thin films*, European Materials Research Society, Spring Meeting 2019, Nice, France, 2019

Talks and Posters

L. von Helden, L. Bogula, P.-E. Janolin, M. Hanke, S. Liang, T. Breuer, R. Wördenweber, M. Schmidbauer, S. Ganschow, and J. Schwarzkopf, *Huge impact of compressive strain on phase transition temperatures in epitaxial, ferroelectric KNN thin films*, Deutsche Physikalische Gesellschaft, Spring Meeting 2019, Regensburg, Germany, 2019

K. Irmscher, A. Fiedler, Z. Galazka, J.B. Varley, *Electron paramagnetic resonance and charge state Transition levels of cobalt in β-Ga_2O_3*, IWGO 19, USA, 2019

N. Jaber, J.E. Boschker, J. Stöver, K. Irmscher, T. Markurt, M. Albrecht, J. Feldl, M. Ramsteiner, J. Schwarzkopf, *structural and electrical properties of NbO_2 epitaxial thin film,* E-MRS 2019, Warsaw, Poland, 2019

S. Kalusniak, A. Uvarova, C. Guguschev, C. Kränkel , *OPTICAL FLOATING ZONE GROWTH OF HIGH-MELTING SESQUIOXIDES,* WODIL2019, Lyon, France, 2019

L. Ladenstein, S. Smetaczek, J. Ring, S. Ganschow, H.M.R. Wilkening, J. Fleig, D. Rettenwander, *Electrochemically active microelectrodes to study locally resolved charge-transfer resistances in solid-state Li batteries,* Joint ISAF-ICE-EMF-IWPM-PFM meeting 2019, Lausanne, Switzerland, 2019

F. Lange, *Progress report on in-plane germanium nanowire growth on nano-patterned substrates*, BTU Graduate Research School: Workshop of Cluster „FuSion" Cottbus, Germany, 2019

R. Menzel, H.-J. Rost, F.-M. Kießling and L. Sylla, *Float-Zone growth of silicon crystals using large area seeding*, GPCCG-3, Poznań, Polen, 2019

R. Menzel, K. Dadzis, A. Nikiforova, N. Lorenz-Meyer, B. Faraji-Tajrishi, N. Abrosimov, H. Riemann, *Growth of Silicon Single Crystals by the Granulate Crucible (SiGC) Method*, 19th International Conference on Crystal Growth and Epitaxy (ICCGE-19), Keystone, USA, 2019

W. Miller, R. Schewski, A. Popp, G. Wagner, M. Albrecht, *A kinetic Monte Carlo model to compute homo-epitaxial growth of Ga_2O_3,* 3rd German Polish Conference on Crystal Growth (GPCCG-3), Poznań, Polen, 2019

N. Modsching, J. Drs, J. Fischer, C. Paradis, F. Labaye, M. Gaponenko, C. Kränkel, V. J. Wittwer, and T. Südmeyer, *Frontiers in high power ultrafast thin-disk lasers operating in the sub-100-fs regime,* Ultrafast Optics Conference XII, Bol, Croatia, 2019

N. Modsching, J. Drs, C. Kränkel, V. J. Wittwer, O. Razskazovskaya, and T. Südmey, *New Horizons for high power broadband THz sources driven by ultrafast Yb-based thin disk laser oscillators,* Conference on Lasers and Electro-Optics (CLEO2019), San Jose, USA, 2019

N. Modsching, J. Drs, J. Fischer, C. Paradis, F. Labaye, M. Gaponenko, C. Kränkel, V. J. Wittwer, and T. Südmeyer, *21 W average power sub-100-fs Yb:Lu2O3 thin-disk laser oscillator*, Conference on Lasers and Electro-Optics (CLEO2019), San Jose, USA, 2019

N. Modsching, J. Drs, J. Fischer, C. Paradis, F. Labaye, M. Gaponenko, C. Kränkel, V. J. Wittwer, and T. Südmeyer, *95-fs Yb:Lu_2O_3 thin-disk laser operating at 21 W average power,* Conference on Lasers and Electro-Optics (CLEO/Europe-EQEC) 2019, Munich, Germany, 2019

A.G. Ostrogorsky, N. Dropka, V. Riabov, *Analysis of heat and mass transfer using rotating baffle in vertical Bridgman configuration*, ICCGE-19 / OMVPE-19 / ISSCG-17, Keystone, USA, 2019

P. Posch, S. Lunghammer, S. Berendts, S. Ganschow, D. Rettenwander, M. Wilkening, *Ion Dynamics in Al-Stabilized $Li_7La_3Zr_2O_{12}$ Single Crystals – Two Elementary Steps of Ion Hopping Seen by NMR,* Joint ISAF-ICE-EMF-IWPM-PFM meeting 2019, Lausanne, Switzerland, 2019

E. Pycha, S. Ganschow, S. Smetaczek, J. Ring, D. Rettenwander, S. Berendts, A.Limbeck, J. Fleig, *Investigating the electrochemical stability of cubic LLZO garnets using field stress experiments*, GÖCH-Chemietage Linz, Linz, Austria, 2019

J. Ring, S. Smetaczek, D. Rettenwader, S. Ganschow, S. Berendts, A. Limbeck, *Impact of field stress on electrochemical prperties of LLZO*, GÖCH-Chemietage in Linz, Linz, Austria, 2019

J. Stöver, A. Fiedler, K. Irmscher, *Deep-Level Transient Spectroscopy*, GraFOx Summer School 2019, Menaggio, Italy, 2019

T. Straubinger, C. Hartmann, L. Mative, J. Wollweber, M. Bickermann, *AlN – Temperature field optimization for low dislocation density after growth and epitaxy*, DGKK-Arbeitskreis Massive Halbleiter, Berlin, Germany, 2019

Talks and Posters

Y. Suhak, P. Fielitz, G. Borchardt, S. Ganschow, K.-D. Becker, D. Roshchupkin, H. Fritze, *Electrical properties of single crystalline Li(Nb,Ta)O_3 solid solutions for high temperature actuator applications,* EUROMAT 2019, Stockholm, Sweden, 2019

A. Suzuki, C. Kränkel, and M. Tokurakawa, *High quality-factor Kerr-lens mode-locked Tm:Sc2O3 laser with anomalous spectral broadening*, 8th Advanced Lasers and Photon Sources Conference ALPS'19, Yokohama, Japan, 2019

A. Suzuki, M. Tokurakawa, C. Kränkel, *High quality factor Kerr-lens mode-locked $TmSc_2O_3$ laser beyond the gain bandwidth limitation,* Conference on Lasers and Electro-Optics (CLEO/Europe-EQEC) 2019, Munich, Germany, 2019

H. Tanaka, D. Schulz, E. Castellano-Hernández, S. Kalusniak, D. Klimm, C.Kränkel, and M. Bickermann, *Terbium-containing fluoride crystals for laser and photonics applications*, 8th French-German Workshop on Oxide, Dielectric and Laser single crystal (WODIL2019), Lyon, France, 2019

T. Teubner, *MBE growth of 28Si layers*, Quantum Tech Meeting: Isotopically enriched Si and Ge for quantum computing, Berlin, Germany, 2019

A. Uvarova, Christo Guguschev, Sascha Kalusniak, and Christian Kränkel, *Growth and characterization of high-melting sesquioxides for 3 µm lasers*, ECLEO conference, Munich, Germany, 2019

A. Uvarova, C. Guguschev, and C. Kränkel, *Growth and characterization of Er3+-doped sesquioxide crystals for 3 µm lasers,* Frühjahrstagung der Deutschen Physikalischen Gesellschaft 2019, Munich, Germany, 2019

A. Uvarova, C. Guguschev, and C. Kränkel, *Optical floating zone growth of high-melting sesquioxides*, 3rd Floating zone techniques workshop, Oxfort, UK

F.Zimmermann, E. Richter, F. C. Beyer, J. Beyer, G. Gärtner, K. Irmscher, I. Gamov, M. Weyers, G. Tränkle, J. Heitmann, *Effects of carbon concentration on the luminescence of GaN*, DGKK-Arbeitskreis Massive Halbleiter, Berlin, Germany, 2019

M. Zupancic, Toni Markurt, Kookrin Char, Young Mo Kim, Youjung Kim, Martin Albrecht, *Origin of the two-dimensional electron gas at the interface between $BaSnO_3$/$LaInO_3$ wide bandgap oxides*, 21st International Conference on Microscopy of Semiconducting Materials (MSM-XXI), Cambridge, UK, 2019

Patents

Patents

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

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

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

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

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

R.-P. Lange, P. Rudolph, M. Ziem
Vorrichtung zur Herstellung von Kristallen aus elektrisch leitenden Schmelzen
(Device for producing crystals from electroconductive 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
Registered Trademark
KRIST*MAG*®

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

Oxides

Z. Galazka, R. Uecker, D. Klimm, M. Bickermann
Method for growing beta phase of gallium oxide (ß-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 Kompositwerkstoff
(Seed holder of a single crystal growth device, single crystal growth device and composite material)
DE102014017021A1

Semiconducting layers

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

Teaching and Education

Membership in Committees

Teaching and Education

HU Berlin

Thomas Schröder, Radhakrishnan Sumathi, Jens Martin
Advanced Crystal Growth for Modern Applications
4 SWS; Humboldt-Universität zu Berlin; SS 2019

Martin Schmidbauer
Röntgenstreuung: Grundlagen und Anwendungen in der Materialwissenschaft
2 SWS; Humboldt-Universität zu Berlin; SS 2019

Martin Schmidbauer
Röntgenstreuung: Grundlagen und Anwendungen in der Materialwissenschaft
2 SWS; Humboldt-Universität zu Berlin; WS 2019/20

Christian Kränkel
Angewandte Photonik
3 SWS; Humboldt-Universität zu Berlin; WS 2019/20

Thomas Schröder, Radhakrishnan Sumathi, Jens Martin
Grundlagen und Methoden der Kristallzüchtung
3 SWS; Humboldt-Universität zu Berlin; WS 2019/20

Detlef Klimm
Phasendiagramme
2 SWS; Humboldt-Universität zu Berlin; WS 2019/20

TU Berlin

Matthias Bickermann
Kristallzüchtung I: Grundlagen und Methoden
2 SWS; Technische Universität Berlin; SS 2019

Matthias Bickermann
Kristallzüchtung II – Methoden und Anwendungen
2 SWS; Technische Universität Berlin; WS 2019/20

BTU Cottbus-Senftenberg

Dietmar Siche
Kristallzüchtung
2 SWS; Brandenburgische Technische Universität Cottbus-Senftenberg; SS 2019

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

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
- NamLab gGmbH Dresden; member of the evaluation committee
- Forschungsverbund Berlin e.V.; Deputy Executive Committee Spokesman (since 11/2019)
- DESY Photon Science Council, member
- microSPIRE (FET project council Uni Milano); member of the advisory committee
- BMBF Quantum Technology – Basics and Application (QuTeGa), member

Conference committees

M. Bickermann
- DGKK Workshop “Bulk Semiconductor Crystals”, Berlin, Germany; conference organizer (with T. Straubinger and R. Sumathi)
- International workshop on UV materials and devices (IWUMD)); program committee member

Z. Galazka
- International Workshop on Gallium Oxide and Related Materials (IWGO-3), Columbus, USA; technical program committee member
- Compound Semiconductor Week 2019 (CSW 2019); Nara, Japan; technical program committee member

C. Guguschev
- ICCGE-19/OMVPE-19, Keystone, USA; program commitee member

Membership in Committees

C. Kränkel
- Solid-state Lasers at Conference on Lasers and Electro-Optics (ECLEO) 2019, Munich, Germany; head of program sub-committee CA
- GPCCG Conference, Poznan, Poland; program committee member
- SPIE Conference 11259, Solid State Lasers XXIX: Technology and Devices; program committee member

W. Miller
- 3rd German Polish Conference on Crystal Growth (GPCCG-3), Poznan, Poland; conference co-chair
- International Conference on Defects-Recognition, Imaging and Physics in Semiconductors (DRIP XVIII), Berlin, Germany; conference organizer (with A. Mogilatenko, FBH), scientific advisory board member13th International Conference on Nitride Semiconductors 2019 (ICNS-13), Bellevue, USA; program committee member

T. Schröder
- Workshop on Dielectrics in Microelectronics (WoDiM), Scientific Advisory Council
- Joint International SiGe Technology and Device Meeting (ISTDM) & International Conference on Silicon Epitaxy and Heterostructures (ICSI), Scientific Advisory Council

T. Straubinger
- DGKK Workshop "Bulk Semiconductor Crystals", Berlin, Germany; conference organizer (with R. Radhakrishhnan Sumathi and M. Bickermann) Modeling Conference in Crystal Growth, SSN, India; scientific advisory committee member

R. Radhakrishnan Sumathi
- DGKK Workshop "Bulk Semiconductor Crystals", Berlin, Germany; conference organizer (with T. Straubinger and M. Bickermann) Modeling Conference in Crystal Growth, SSN, India; scientific advisory committee member

Editoral 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

Other Committees

M. Bickermann
- Best poster award, Adlershofer Forschungsforums 2019, member of the jury

T. Schröder
- Humboldt Universität Berlin: Director Paul Drude Institut; member of the appointment committee
- Brandenburgisch Technische Universität Cottbus – Senftenberg: wireless systems; member of the appointment committee
- Leibniz Association project group on gender equality and management college on „Equality and Reconciliation"; member

Guest Scientists

Guest Scientists

Marianne Lado-Roy
16.01. – 18.01.2019
Polytechnique Montréal
Canada

Prof. Dr. Oussama Moutanabbir
16.01. – 18.01.2019
Polytechnique Montréal
Canada

Prof. Kookrin Char
21.01. – 15.02.2019
18.07. – 07.08.2019
Seoul National University
South Korea

Prof. Dr. Darrell G. Schlom
01.02. – 31.05.2019
Cornell University
USA

Dr. Philip Weiser
18.02. – 22.02.2019
University of Oslo
Norway

Dr. Humberto Foronda
01.03.2019 – 31.05.2021
"Forschungsstipendiat
Alexander von Humboldt-Stiftung"

Dr. Andrejs Sabanskis
13.05. – 24.05.2019
University of Latvia
Latvia

Prof. Sven Rogge
18.06. – 27.06.2019
University of New South Wales
Australia

Prof. Dr. Niu Gang
01.07. – 29.07.2019
Xi´an Jiaotong University
China

Prof. Dr. Petr G. Sennikov
01.07. – 31.08.2019
Russian Academy of Sciences
Russia

Chen Ling
15.07. – 13.08.2019
Peking University
China

Wang Tao
15.07. – 13.08.2019
Peking University
China

Colloquia at the IKZ

Colloquia at the IKZ

Prof. Dr. Oussama Moutanabbir
"Isotopically Programmed Group IV Semiconductors: A Versatile Platform for Quantum Technologies"
Polytechnique Montréal, Technological University, Department of Engineering Physics
Montreal, Canada
January 18, 2019

Prof. Dr. Thomas Mikolajick
"Ferroelectricity in Hafnium Oxide: Basics and Applications"
Technische Universität Dresden, Institut für Halbleiter- und Mikrosystemtechnik;
NaMLab gGmbH Dresden, Germany
January 28, 2019

Dr. Daniel Rettenwander
"The interplay of ionic conductivity and crystal chemistry in ceramic electrolytes for all solid-state batteries"
Technische Universität Graz, Institut für Chemische Technologie von Materialien
Graz, Austria
February 11,2019

Dr. Markus R. Wagner
"Excitions, phonons, and thermal transport in Ga_2O_3 polymorphs"
Collaborative Research Center 787 "Semiconductor Nanophotonics"
Technische Universität Berlin, Institut für Festkörperphysik
Berlin, Germany
February 18,2019

Prof. Dr. Andreas Stierle
"Atomic structure of oxide surfaces and ultrathin oxide films"
Forschungszentrum der Helmholtz-Gemeinschaft, Deutsches Elektronen-Synchrotron DESY
Hamburg, Germany
February 19, 2019

Dr. Daniel Fritsch
"Self-consistent hybrid functionals: Implications for structural, electronic, and optical properties of oxide semiconductors"
Helmholtz-Zentrum Berlin für Materialien und Energie GmbH
Berlin, Germany
February 25, 2019

Prof. Dr. Oleg Pronin
"Femtosecond oscillators based on Yb:YAG, Ho:YAG, Cr:ZnS/Se gain media and broadband infrared generation in LGS, GaSe, ZGP nonlinear crystals"
Helmut-Schmidt-Universität/Universität der Bundeswehr Hamburg
Hamburg, Germany
March 01, 2019

Dr. Ausrine Bartasyte
"$LiNbO_3$ thin films for next generation acoustic filter applications"
Universitè de Franche-Comté, Institut-FEMTO-ST
Besançon, France
March 12, 2019

Dr. Vincenzo Grillo
"Quantum experiments in electron microscopy"
University of Modena, CNR NANO, Institute of Nanotechnology
Modena, Italy
March 18, 2019

Prof. Dr. Bernd Witzigmann
"Carrier Injection Efficiency and Impurity Modelling in III-nitride LEDs"
Computational Electronics and Photonics
Universität Kassel, Fachbereich Elektrotechnik/Informatik
Kassel, Germany
April 01, 2019

Prof. Dr. Thorsten M. Gesing
"Bismuth ferrates and tungstates: thermal expansion and materials size dependent properties"
Universität Bremen, Anorganische Chemie
Bremen, Germany
May 06, 2019

Dr. Humberto Foronda
"Achieving Grain Free (11-22) AlGaN/AlN surfaces on m-plane sapphire"
Alexander von Humboldt Fellow at Technische Universität Berlin and IKZ
Berlin, Germany
May 20, 2019

Dr. Janis Virbulis
"Modelling of silicon crystal growth"
University of Latvia, Laboratory for Mathematical Modelling of Environmental and Technological Processes
Riga, Latvia
May 21, 2019

Colloquia at the IKZ

Prof. Dr. Alois Lugstein
"Synthesis and applications of quasi 1D metal-semiconductor nanowire heterostructures"
Technische Universität Wien,
Zentrum für Mikro- und Nanostrukturen
Vienna, Austria
June 03, 2019

Dr. Jens Martin
"Layer Transfer: A Technology for Novel 2D-Hetero-Structures"
IKZ, Physikalische Charakterisierung
Berlin, Germany
June 24, 2019

Prof. Dr. Gérard Aka
"Growth of oxide crystals for lasers and other optical applications"
Chimie ParisTech
Paris, France
July 29, 2019

Dr. Michael Beck
"Optical spectroscopy of donor bound excitons and spin relaxation of donor electrons in isotopically enriched silicon"
Leibniz Universität Hannover, Institut für Festkörperphysik, Abteilung Nanostukturen
Hannover, Germany
September 10, 2019

Prof. Dr. Norbert Esser
"VUV-Ellipsometry with Synchrotron Radiation: High-Resolution Broadband Analysis of Wide-Bandgap-Semiconductors"
Leibniz-Institut für Analytische Wissenschaften (ISAS), Forschungsbereich Grenzflächenanalytik
Berlin, Germany
September 16, 2019

Prof. Dr. Andreas Klein
"Fermi level and performance limits of oxides"
Technische Universität Darmstadt,
Elektronenstruktur von Materialien
Darmstadt, Germany
September 17, 2019

Prof. Dr. Stefanie Kroker
"Crystalline bulk materials and meta-surfaces for high-precision experiments – status, prospects and challenges"
Technische Universität Braunschweig,
LENA Laboratory / Physikalisch-Technische Bundesanstalt
Braunschweig, Germany
September 23, 2019

Prof. Dr. Detlev Grützmacher
"Modern Epitaxy and Devices for Advanced Information Technology"
Forschungszentrum Jülich, Peter Grünberg Institut, Halbleiter-Nanoelektronik
Jülich, Germany
September 30, 2019

Dr. Vincent Fratello
"Congruently Melting Perovskite Solid Solutions"
Quest Integrated, Materials Research
Kent, WA, USA
October 07, 2019

Prof. Dr. Christian Teichert
"Growth of organic semiconductor nanocrystals on two-dimensional materials"
Montanuniversität Leoben, Institut für Physik
Leoben, Austria
October 11, 2019

Dr. Tim Schröder
"Diamond – Exciting resource for Quantum Technology"
Humboldt-Universität zu Berlin, Institut für Physik
Berlin, Germany
October 21, 2019

Prof. Dr. Roman Engel-Herbert
"Complex oxides"
Penn State University,
College of Earth and Mineral Science
State College, PA, USA
November 01, 2019

Prof. Dr. Yadong Xu
"The progress on semiconductor bulk crystals for nuclear radiation detection in NPU"
Northwestern Polytechnical University,
Key Laboratory of Radiation Detection Materials and Devices
Xi'an, China
November 06, 2019

Colloquia at the IKZ

Dr. Gudrun Kissinger
"On the impact of deposited oxide and nitride layers on oxygen precipitation in silicon"
Leibniz-Institut für Innovative Mikroelektronik (IHP), Materials Research/Adaptive Materials
Frankfurt/Oder, Germany
December 02, 2019

Prof. Dr. Ulrich Theodor Schwarz
"(Al,In)GaN laser diodes dynamics from nanosecond to millisecond range"
Technische Universität Chemnitz, Institut für Physik
Chemnitz, Germany
December 16, 2019

Prof. Dr. Mathias Schubert
"Strain, stress, alloying and defects in monoclinic gallium oxide and related compounds: Determination of phonon, free charge carrier, band gap and defect properties with THz Electron Paramagnetic Resonance, Optical Hall effect and ultra-wideband generalized ellipsometry".
University of Nebraska-Lincoln,
Nebraska Center for Materials and Nanoscience
Lincoln, NE, USA
December 20, 2019

Leibniz-Institut für Kristallzüchtung (IKZ)
Director: Prof. Dr. Thomas Schröder
Max-Born-Straße 2
12489 Berlin
Germany

Phone +49 (0)30 6392 3001
Fax +49 (0)30 6392 3003
Email cryst@ikz-berlin.de
Online www.ikz-berlin.de

Annual Report 2019

Editors: Dr. Maike Schröder and Lisa Picard

Layout & typesetting: www.typoly.de

Print: www.katalogdruck-berlin.de

Cover photo:
„Ausschnitte der Si-Kugel aus dem Züchtungskristall in IKZ-Züchtungshalle“ –
“Sections of the Si-sphere from the growing crystal in the IKZ growth hall”
A. Riemann

Berlin, September 2020

Leibniz-Gemeinschaft

Leibniz-Institut für Kristallzüchtung (IKZ)

Max-Born-Straße 2
12489 Berlin
Germany

Phone +49 (0)30 6392 3001
Fax +49 (0)30 6392 3003
Email cryst@ikz-berlin.de

www.ikz-berlin.de