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







## Dear Readers,

The Leibniz-Institut für Kristallzüchtung (IKZ) is the European flagship institute for research & development (R&D) in the field of crystalline materials and related technologies.

Together with national & international partners from academia as well as industry, we cover the full research spectrum from basic over applied science up to pre-industrial development.

> It is our pleasure to welcome you at our institute and feel free to contact us for further information.





Prof. Dr. Thomas Schröder Director of the Institute



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Crystalline layers and nanostructures are key elements for applications e.g. in microelectronics, sensor technology, data storage, photovoltaics or quantum technology. They provide defined functionalities through precisely adjustable physical properties in the films itself, but also by using sequences of layers, or through modification of the crystalline structures on the micro- or nano scale. The rather unique synergy of in-house growth of substrates with the epitaxy of crystalline layers provides us with the best conditions for research and development of new functional materials with tailored properties.

> Our scientific mission focuses on the investigation of innovative crystallization methods, fundamental growth mechanisms and the relation between structure and function. The material spectrum comprises mainly oxide layers and semiconductors, among them isotopically pure or enriched germanium-76 or silicon-28 for quantum technology.

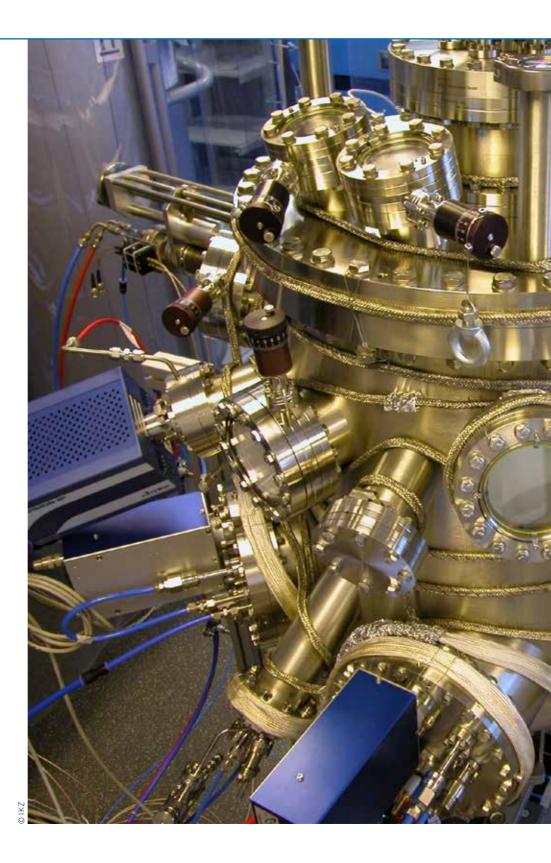
# Nanostructures & Layers

#### Semiconductor Nanostructures

Crystalline structures on the micro- or nanoscale are at the heart of innovative technologies, such as nano- and quantum technology. Our research activities focus on the growth of highly functional materials with applications in microelectronics, photovoltaics or quantum technology. This comprises for example nanowire growth for new field-effect transistors, micro-island generation and thin-film growth from solution for solar applications as well as deposition of ultra-thin strained layers for the use in quantum computers. Not only **technology development and characterization, but also concepts and realization of novel growth systems or components, also in cooperation with industry**, are in our focus.

The defined patterning of crystalline structures on the nano- and microscale is one prerequisite for their application in innovative devices. Therefore, we investigate growth mechanisms and local control of nano- and microcrystallites and develop methods for their implementation.

One of our main topics is the research on isotopically pure or enriched materials for quantum computing. Qubits can be formed in high-quality strained layers embedded in semiconductor heterostructures. Especially silicon-28 and germanium-76 are very promising candidates, because they have a very high scalability and devices could be fabricated using already existing technologies.



We research innovative materials for quantum- and nanotechnology, from basic research to technology development. One focus is on isotopically pure or enriched semiconductors like silicon and germanium.

#### Thin Oxide Films

Oxides are very versatile, since their physical properties can be adjusted by composition, doping or even controlled strain incorporation in thin layers. Therefore, they are ideal candidates for **a wide range of (new) applications, like in oxide electronics.** They allow to realize devices with higher switching speed or storage densities, but with smaller dimensions or less energy consumption than conventional ones. In addition, they have the potential to replace lead-containing compounds still used in common electronic devices today with more environmentally friendly technologies.

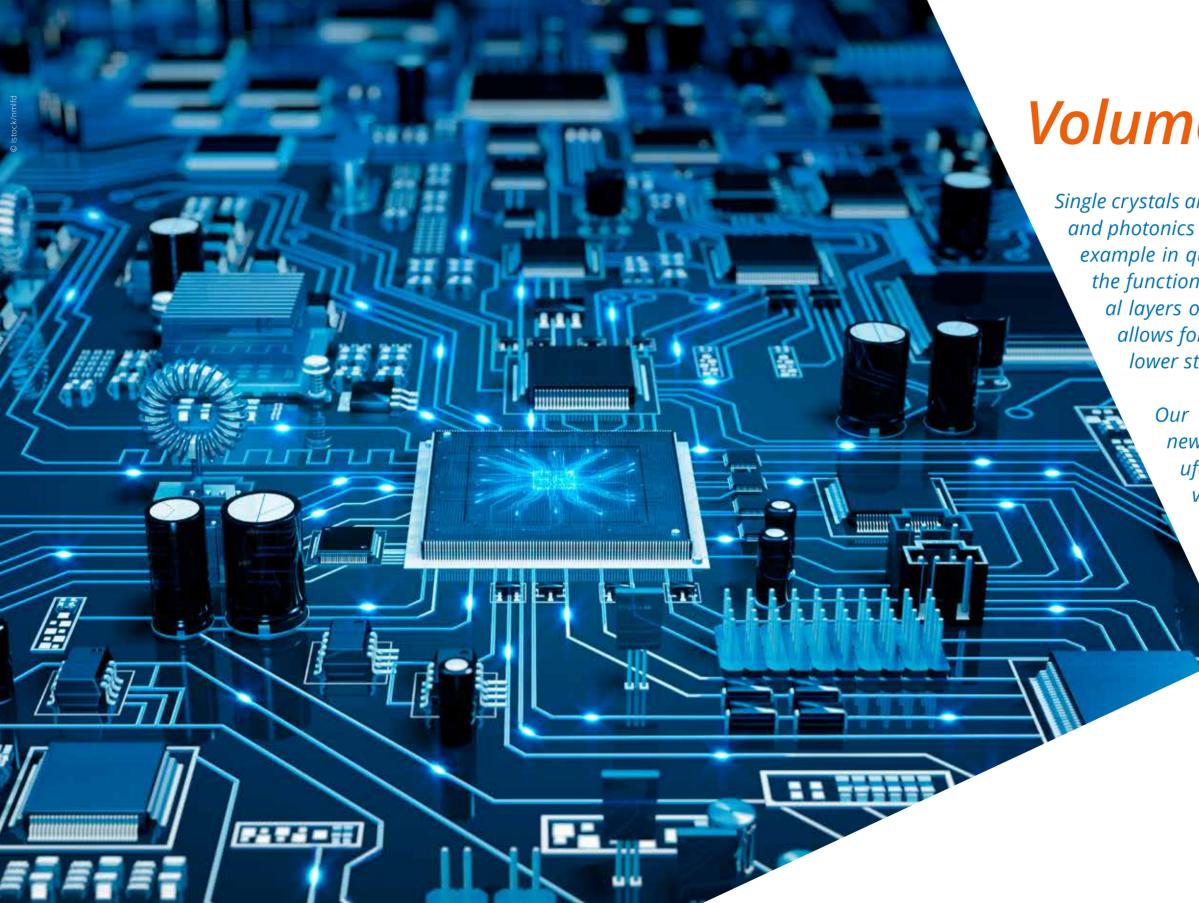
#### The unique combination of substrate and layers we

have in-house opens an additional degree of freedom: on the one hand, the intended mismatch between them could be used to specifically induce strain in the layers, leading to special properties which are not present in the relaxed material. On the other hand, layers of very high quality may be achieved by homoepitaxy, i.e. deposition on a substrate of the same material and composition. This high perfection opens up areas of application that would not be achievable with lower quality material. In addition, the physical properties of these layers can be precisely adjusted by doping. We focus our research on a deeper understanding of growth mechanisms to prepare layers with **tailored semiconducting**, **dielectric or ferro-/piezoelectric specifications.** Methods in use are the metal-organic vapor phase epitaxy MOVPE or pulsed laser deposition PLD.

Layer transfer is a new scientific approach we are evaluating for the preparation of crystalline materials. Here, thin layers are transferred to foreign substrates instead of deposited directly on them. Since the quality of the layers does not depend on the substrate material, this opens the access to substrate/layer combinations which could not be achieved using conventional growth methods. These new heterostructures could be used for innovative applications in electronics and photonics.







# Volume Crystals

Single crystals are – literally – the basis for modern technologies in electronics and photonics as well as a starting point for innovative developments as for example in quantum technology. Their physical properties are crucial for the functionality of devices – as substrate for the deposition of functional layers or as bulk material. In addition, a high crystalline perfection allows for applications that would not be achievable with materials of lower structural quality.

> Our core competencies comprise research and development of new and innovative materials as well as of corresponding manufacturing technologies, from basic research to industrial-relevant optimization of growth methods for already established materials.

> > We cover a wide range of materials and as a scientific service institute, we also offer the growth of special crystals for research or as reference materials.

Our expertise in semiconductors comprises the development of industry-related manufacturing processes as well as the growth of customized crystals with the highest perfection for research and development.

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We research on **semiconductor single crystals for modern applications in micro- or power electronics, high frequency- or quantum technology**. From the materials side, our focus is on classical group-IV or III-V semiconductors like gallium arsenide or indium phosphide.

Our aim is to grow these materials with the highest possible perfection and to develop corresponding growth methods. This comprises the further development of conventional processes for already established materials up to pre-industrial scale, often in co-operation with partners from industry. Our in-house expertise on numerical modelling and on construction allows us to efficiently modify and improve conventional growth processes and methods. For example, several of our crystal growth units are equipped with the KristMag® technology developed in-house which improves the crystal growth of semiconductors by applying magnetic fields.

#### Crystals with highest perfection and purity are also **key** elements for basic research and can help to answer fundamental questions of physics or chemistry.

For example, isotopically enriched germanium crystals can help to resolve the fundamental properties of neutrinos and thus give insight into the origin of matter in the universe. In addition, the most perfect crystal spheres with highest purity from isotopically pure silicon-28 were used to determine the exact value of the Avogadro constant – a fundamental value in chemistry. Only then it was possible to define the kilogram mass unit based on natural constants which came into effect in 2019.

#### **Oxides & Fluorides**

Optoelectronic and photonic devices, isolators, sensors or lasers are just some of the typical applications for oxide and fluoride single crystals. Especially oxides with their wide range of possible compositions and resulting physical properties are perfectly suited for the development of new and innovative technologies. This includes for example the upcoming field of oxide electronics, which aims to surpass the conventional semiconductor-based CMOS technology by new materials with tailored properties.

#### The functionality of electronic or photonic devices relies substantially on the crystalline quality of their functional

**layers** which in turn is determined by the substrates they are deposited on. Therefore, we grow substrate crystals with tailored properties for different applications. With our in-house expertise on growth of substrate materials as well as epitaxy of crystalline layers we have unique possibilities for the development of innovative material systems with adjustable properties.

Oxides and fluorides are also employed as laser materials, frequency converters, optical isolators or optical windows. In close co-operation with the **Center for Laser Materials at the IKZ**, we research and develop new materials up to prototype level.

Last but not least, oxide crystals of high structural perfection and purity are welcome by researchers and adopters worldwide as reference and test materials, e.g. for geology, solid state physics, scintillator, battery and energy research.





Due to our long-standing experience in growing crystals for various applications, our service ranges from exploration of new materials to development and provision of customized crystals and growth techniques. The Materials Science at IKZ is aiming at solving fundamental scientific questions in the physics of crystalline solids and crystal growth by using experimental characterization as well as numerical modelling. These insights significantly contribute to the research and development of new materials or technologies.

Our research activities focus on the relationship between the crystalline structure of materials and their chemical and physical properties. By enlightening the mechanisms leading to the formation of interfaces, phases or defects, we help to improve crystal growth processes and thus the perfection of crystalline materials, thus opening perspectives for their possible application. For this purpose, we employ a broad range of characterization techniques as well as numerical modeling.

In addition, we investigate methods of artificial intelligence and machine learning which may play an increasingly important role both for pattern recognition in characterization as for modeling and process control.

## **Materials Science**





#### Experimental Characterization

We utilize a **comprehensive spectrum of characterization tools** to investigate materials grown at the institute or at partners from research and industry. These methods comprise **structural**, **optical**, **electrical and thermoanalytical techniques**, **covering macroscopic to atomic length scales**. Doping, atomic defects, the structure of epitaxial heterostructures, growth and relaxation phenomena as well as optical properties are the most important topics of our investigations, with the material portfolio focusing mainly on semiconductors and dielectrics.

Beyond the scientific service we provide to the growth groups, we also perform research on the fundamental structure-property relationship of crystalline materials. This includes, among other things, the analysis of defects which may influence the optical or electrical properties of semiconductors and devices based on them. Transport and capacitive measurements will give information on the electrical conductivity which is important for semiconductor devices in modern electronics. Measurements include the concentration and mobility of free charge carriers, dopants, or compensating impurities.

In addition, we are **developing characterization methods such as in-situ techniques in transmission electron microscopy and x-ray diffraction** with the latter performed in-house as well as at modern synchrotron facilities like BESSY, DESY or ESRF. This enables us to gain a deeper insight into dynamics at atomic resolution or into phase transitions in crystal structures, for example during growth or under the influence of external fields.

#### **Fundamental Description**

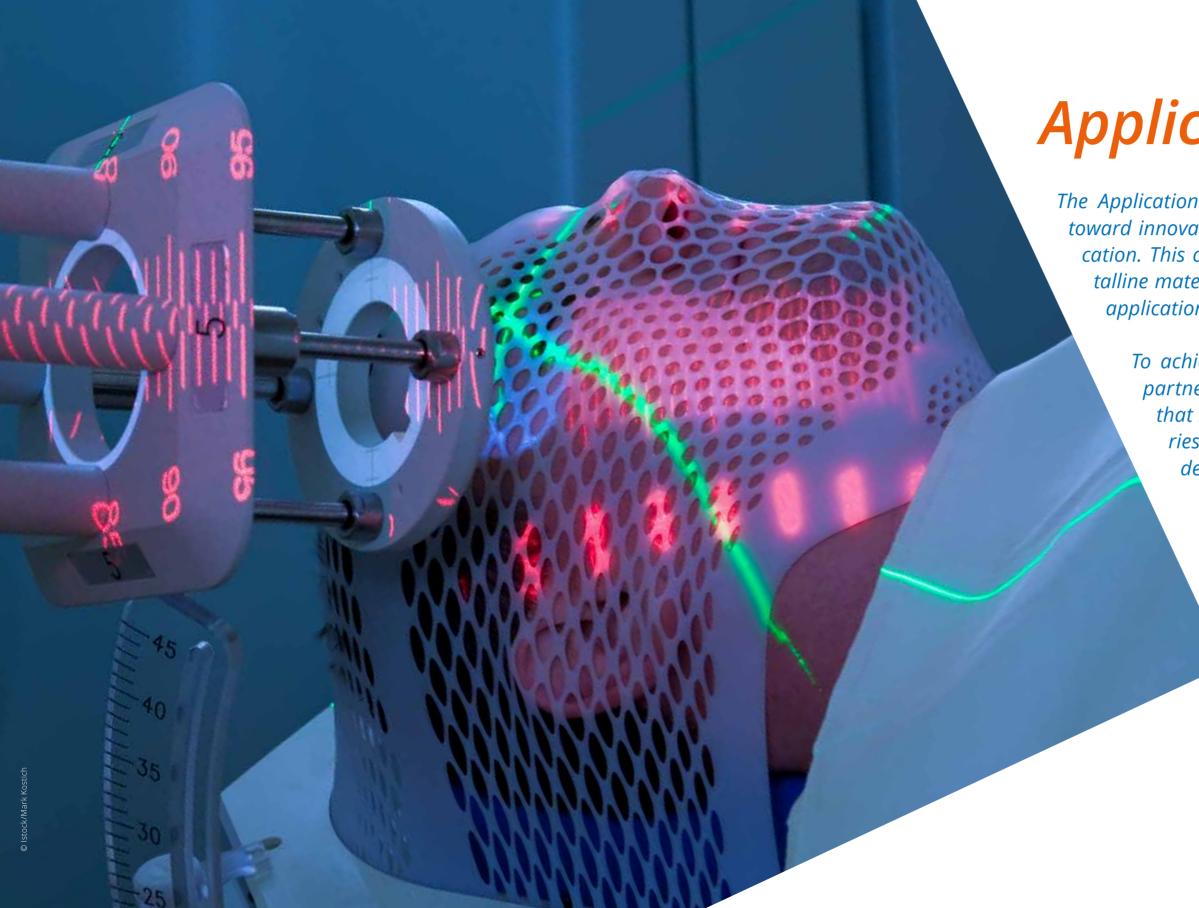
Numerical simulation is an effective tool to understand crystal growth processes by providing a deeper insight in the underlying growth mechanisms. These complex high-temperature processes involve a large variety of physical phenomena such as heat transfer or fluid dynamics. To include this complexity of phenomena in the simulations, we are working on a new generation of multiphysical models. The expected paradigm change in the way how we observe, describe and develop crystal growth processes will minimize the necessary experimental cycles and open new horizons for scientific analysis as well as for smart process control using artificial intelligence and other modern technologies.

Our research activities range from fundamental research – such as on growth kinetics on atomic level – up to applied science on industrial scale. The simulation of temperature and flow fields in crystal growth furnaces, of thermal tensions in the crystal-melt phase boundary or the crystals themselves help to effectively optimize growth processes using a systematic and cost-efficient approach. This includes also the design of growth equipment or components in co-operation with our in-house construction group as well as the control of growth processes using artificial intelligence. Besides the close co-operation we have to the growth groups in-house, we also provide our services, including feasibility studies, to external partners.





Simulation helps to understand both processes on atomic scale and in complex systems like crystal growth, also using methods such as artificial intelligence. Our in-house expertise allows us to modify and construct crystal growth equipment.

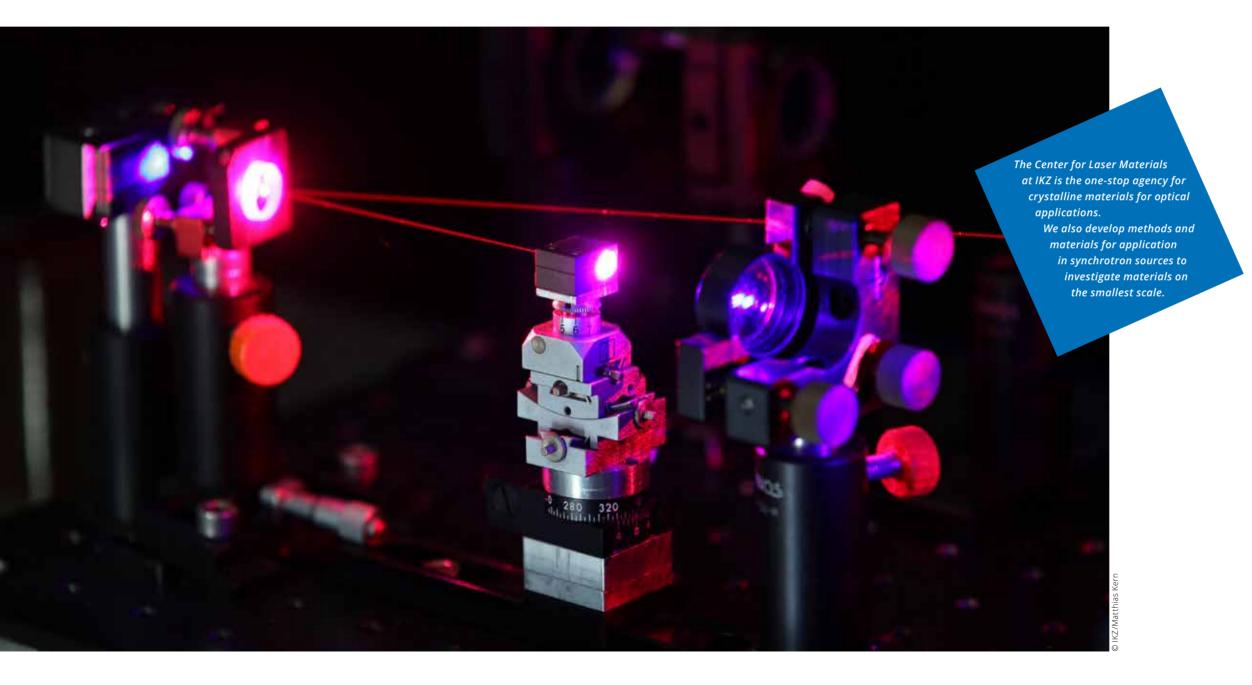


# **Application Science**

The Application Science at IKZ aims at extending the value chain at IKZ toward innovation by crystalline materials, serving as interface into application. This comprises the research and development of innovative crystalline materials that exhibit a high potential for future innovations and applications in electronics or photonics.

To achieve this, we provide prototypes with defined properties to partners in research and industry. We develop reliable processes, that reproducible yield the required specifications, up to small series production. This builds a reliable basis for our partner to develop devices based on our crystals.

> Not only the development of materials plays an essential role on the way into application, but also the preparation of substrates for epitaxy. In this way we make our in-house grown crystals available to partners for further research and development.



#### Crystalline Materials for Photonics

The Center for Laser Materials is dedicated to research and qualification of crystalline materials for optical ap-

**plications.** The center serves as international one-stop shop for partners from research and industry for optical crystals for laser applications, optical isolators or non-linear frequency conversion. Our research covers **crystal growth of laser materials, characterization and assembling** including the combination with matching pump laser diodes or modules as well as testing. Our main focus lies on rare earth and transition metal doped oxide and fluoride crystals that may open up new wavelength ranges, enable more efficient laser operation or higher output power.

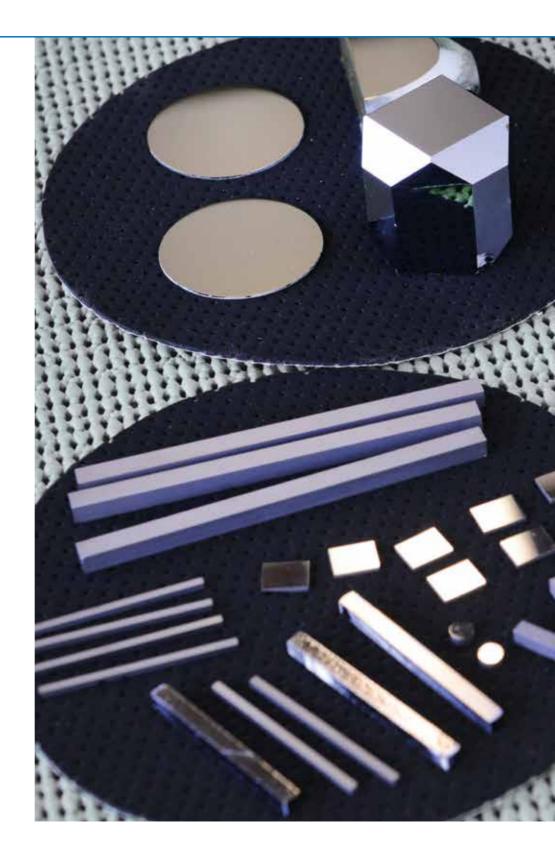
Another focus of our scientific activities is the **development** of optical components and methods to control hard x-rays for application in synchrotron radiation sources. This allows us to adapt the parameters of the emitted beam to the individual experiment and to perform studies on smallest dimension and time scales, such as x-ray imaging of nanoscale integrated circuits or the dynamics of crystalline materials by time-resolved x-ray methods. Besides developing such optics, we also investigate the influence of the crystal structure on the electrical, optical or magnetic properties of the material.

#### Crystalline Materials for Electronics

Our mission is to enable innovations by crystalline materials and to bring them into application. Therefore, we try to **identify the most promising materials from our research portfolio and take them from basic research to the production of prototypes.** Focusing on semiconductor materials for electronic applications, we optimize and develop growth and preparation processes for small-scale production of **crystalline materials with high and reliable quality and well-defined specifications.** This in turn enables our partners from technology-oriented research institutes or from industry to develop new devices or fabrication processes.

A key element in technology development is the availability of high-quality substrates as basis for the deposition of crystalline layers. In addition to the specific properties, also the quality of these layers or following sequences of them determine the functionality of electronic devices and eventually also the range of possible applications. We develop **material-specific methods for processing crystals, including low-loss sawing of materials according to their different mechanical properties, polishing of wafers with high quality surfaces as well as precise crystallographic orientation**.

In addition, we use **chemical analysis** to determine impurities on the wafer surface, but also to analyze the starting materials for our growth experiments in terms or impurities and chemical composition. This allows us to compare the results from our growth runs and exclude or evaluate these influences with respect to crystal quality.



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We offer small scale series of epi-ready substrates with defined properties for device development to potential partners from industry and research. One key element here is our expertise in crystal preparation. We are committed to bring our research and material into application. Moreover, we have a dedicated mission to offer scientific services to research institutions and industry. This includes research on new crystalline materials as well as technology and process development, but also our expertise in characterization, equipment development, crystal processing and modeling.

Our offers comprise research and development in joint projects, as well as commissioned research. Besides the growth of (non-commercial) crystals, our services also include feasibility studies, expert opinions, as well as training and workshops on demand.

The major research topics of the institute is covered by our patent portfolio, which we use as a basis for start-ups or offer for licensing to interested companies.

# **Transfer and Service**



#### **Our Portfolio**

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Development of new devices or future technologies requires not only high-quality crystalline materials with tailored properties, but also their reliable availability. Our aim is to go beyond the academic level, offering partners **small-scale series of material with reproducible properties** and thus enabling them to develop new technologies or devices based on them. This will enable not only innovations in but also by crystalline materials.

Together with our scientists, research partners and industrial collaborators we identify and secure potential innovations and stimulate and accompany their commercial exploitation. **Licenses** entitle you to use our comprehensive, proprietary, technical know-how, which is constantly expanding and can lead to new products and innovative processes. The type and scope of the licenses are varying, as well as their form that can be agreed upon individually.

Our services include all areas of our research portfolio, including material research and development, characterization, crystal preparation or construction of growth equipment. We provide feasibility studies and expert opinions on material science topics. In addition, we are also offering individual workshops and training courses on demand.

as services such as characterization, simulation or preparation. Contact us if you are interested in research co-operations or licensing of our patent portfolio. 0



#### Contact us



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#### LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG im Forschungsverbund Berlin e.V

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Max-Born-Straße 2 12489 Berlin

www.ikz-berlin.de

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LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG im Forschungsverbund Berlin e.V

Max-Born-Straße 2 12489 Berlin

www.ikz-berlin.de