DKT 2020

dgkk

Deutsche Kristallzüchtungstagung
11.-13. März 2020 in München/Garching

50 Jahre Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung e. V.

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Editoral

A warm welcome to everybody to the Annual German Crystal Growth Conference ("Deutsche Kristallzüchtungstagung, DKT 2020") of the German Association of Crystal Growth DGKK (Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung e. V.) !

This year we are happy and proud to celebrate the 50th anniversary of DGKK. It was founded in April 1970 and later in October the first general assembly took place in Munich together with the colloquium "Kristallzüchtung" of the German Research Foundation (DFG). With actually just nearly 400 individual and institutional members, the DGKK is an important part of the crystal growth community in Europe and well connected worldwide. From the very beginning until today the success of the association is based on the interdisciplinarity of the members coming from all fields of natural sciences and engineering and united in the complexity of the single crystal growth and the cutting edge technology needed. Such a widespread collection of interests and topics, all focusing on structural perfection, optimum performance for technical applications, unique physical properties and last not least in the aesthetic and beauty of crystals may be unique. The DGKK combines and promotes all of the fundamental and applied knowledge in crystal growth science and technology, which is documented in the special issue of the Journal Crystal Research & Technology Vol 55(2) 2020, dedicated to the 50th Anniversary of the German Association for Crystal Growth and this book of extended abstracts. It mirrors our very active crystal growth community and our vital working groups in all its facets. Certainly the retrospection on occasion of our commemorative session on Thursday afternoon followed by the gala dinner is the central event and we wish at this place to express our thanks to all our members for their unwearied efforts to boost our community all the years. We are pleased to welcome some of the merited "veterans" of the very first years and we would like to express our thanks and very best wishes to all of our fellows, who cannot join our celebration because of health reasons.

Beside the look back, the future perspectives are our central concern for the DKT 2020. The talks given by former and actual laureates of the DGKK prize as well by the invited speakers are supposed to inspire our discussion about our future challenges ranging from basic research, new materials and complex engineering technology to new computing methods and artificial intelligence.

Finally we would like to express our gratitude to all the institutions and companies named on the front cover for generous financial support. We wish you all a fruitful and unforgettable conference and look ahead a successful future of our DGKK,

Andreas Erb, Wolfram Miller, Andreas Danilewsky

Grußworte der Vorsitzenden des Exzellenzclusters ORIGINS

Liebe Mitglieder der DGKK,

im Namen der Mitglieder des Münchner ORIGINS Clusters gratulieren wir ganz herzlich der DGKK zum 50-jährigen Jubiläum.

Der Exzellenzcluster ORIGINS untersucht die Entstehung des Weltalls und den Ursprung des Lebens. Er geht aus der sehr fruchtbaren Zusammenarbeit zwischen Astro-, Teilchen- und Kernphysikern innerhalb des vorherigen Exzellenzclusters Universe hervor, der die grundlegenden Eigenschaften des Universums erforschte. Hochreine Kristalle spielen hierbei eine ganz wichtige Rolle: sie werden zur Suche nach der dunklen Materie verwendet, zum Nachweis von Neutrinos bei niedrigsten Energien, zur Spurensuche was mit der anfänglichen Anti-Materie im Universum geschehen ist, oder um die Kopplung von hypothetische Teilchen an Photonen zu vervielfachen. Grundlagenforschung in der Kern-, Astro- und Teilchenphysik und Kristallwachstum sind eng mit einander verbunden und die aktuelle Forschung in einem der Forschungsfelder beflügelt oft das andere.

Wir wünschen Ihnen eine erfolgreiche Jahrestagung 2020!

Herzliche Grüße
Ihr

Prof. Stephan Paul Prof. Andreas Burkhart

Co-Sprecher des Exzellenzcluster ORIGINS, München

Deutsche Gesellschaft für Kristallographie

Grußwort vom Vorsitzenden der DGK

Liebe Mitglieder der DGKK,

im Namen der Deutschen Gesellschaft für Kristallographie gratulierte ich der DGKK ganz herzlich zu ihrem 50-jährigen Bestehen. Kristallzüchtung und Kristallwachstum haben in den 50 Jahren nicht an Bedeutung verloren, im Gegenteil, manche Fragen sind heute aktueller sind denn je.

Die DGKK und die DGK sind nicht nur durch ihre ähnlichen Namen verbunden, sondern auch durch gemeinsame wissenschaftliche Interessen, wie z.B. in den Materialwissenschaften. Dies spiegelt sich auch in gemeinsamen Aktivitäten wieder, wie ein gemeinsam organisiertes Mikrosymposium im Rahmen der DGK Jahrestagung 2018 sowie in 2019 beim GPPCG-3 in Poznań und einer DGK Summer School in Mühlheim, denen in Zukunft hoffentlich weitere gemeinsame Veranstaltungen folgen werden.

Ich wünsche Ihnen eine erfolgreiche Jahrestagung 2020!

Herzliche Grüße
Ihr

Ralf Ficner
Georg-August-Universität Göttingen
Vorsitzender der DGK

DGM 1919-2019 100 Jahre Innovationen

Deutsche Gesellschaft für Materialkunde e.V.

DGM · Deutsche Gesellschaft für Materialkunde e.V.
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An die

Deutsche Gesellschaft für
Kristallwachstum und Kristallzüchtung e.V.

12. Januar 2020

Grußwort zu 50 Jahre DGKK

Manche Erfindungen verdanken sich dem glücklichen Zufall. Als Jan Czochralski 1913 beim Verfassen seines Tagesberichts im Metall-Forschungslabor der AEG seine Feder statt in die Tinte in die heiße Zinnlösung für seine Experimente tauchte, entdeckte er, wie man einen Einkristall aus einer Zinnschmelze zieht: eine neue Methode zur Herstellung von einkristallinen Werkstoffen. Das Czochralski-Verfahren ist heute eines der wichtigsten Züchtungsverfahren – und damit von großer Bedeutung nicht nur für die Metallurgie, sondern in besonderem Maße auch für die Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung e.V. (DGKK), deren 50. Geburtstag wir 2020 feiern können.

Im vergangenen Jahr wurde die Deutsche Gesellschaft für Materialkunde e.V. (DGM) 100 Jahre alt – und Jan Czochralski war eines ihrer Gründungsmitglieder! Über seinen Namen und sein Wirken sind die beiden Gesellschaften also seit rund einem halben Jahrhundert miteinander verbunden – eine Verbindung, die durch die Zusammenarbeit in der Bundesvereinigung MatWerk längst auch praktischen Nutzen für DGKK und DGM nach sich gezogen hat.

In diesem Sinne ist es uns eine große Freude, der DGKK hiermit herzlich zu ihrem runden Jubiläum zu gratulieren. Die von ihr geförderte Forschung, Lehre und Technologie auf den Gebieten Kristallwachstum, Kristallzüchtung und Epitaxie etwa durch Ausbildungs- und Fortbildungsveranstaltungen hat auch auf die von der DGM vertretenen Bereiche der Materialwissenschaft und Werkstofftechnik zurückgewirkt. Auch ihre erfolgreiche Nachwuchsförderung hat uns immer wieder sehr beeindruckt.

Wir freuen uns im Namen unserer Mitglieder auf die weitere gemeinsame Zukunft.

Mit freundlichen Grüßen

F. Mücklich

Prof. Dr.-Ing. Frank Mücklich
Präsident der Deutschen Gesellschaft für Materialkunde e.V.

O. Schauerte

Dr. Oliver Schauerte
Präsident der Deutschen Gesellschaft für Materialkunde e.V.

Grußwort zum 50-jährigen Bestehen der Deutschen Gesellschaft für Kristallwachstum und Kristallzüchtung e.V. (DGKK)

Dr. phil. nat. Ursula Eul

Bundesvereinigung Materialwissenschaft und Werkstofftechnik e.V. (BV MatWerk)
E-mail: vorstand-bv@matwerk.de

Zu ihrem 50-jährigen Bestehen gratuliert die Bundesvereinigung Materialwissenschaft und Werkstofftechnik e.V. (BV MatWerk) der Deutschen Gesellschaft für Kristallwachstum und Kristallzüchtung e.V. (DGKK) sehr herzlich.

Hochwertige Kristalle halfen in der präparativen Chemie der 1950er Jahre, das Rätsel unserer Erbsubstanz zu lösen. Ohne technische Kristalle gäbe es heute weder WLAN noch Laser Pointer, weder Ultraschall-Gerät noch Körperscanner. Siliziumkristalle bilden die unverzichtbare Materialbasis für die Halbleiterindustrie und für die Solarindustrie. Ohne die wissenschaftlichen und technischen Erfolge in der Kristallographie wäre unsere Welt heute nicht so, wie sie ist.

In den 50 Jahren ihres Bestehens hat die DGKK mit ihrem Einsatz für Forschung, Lehre und Technologie von Kristallwachstum, Kristallzüchtung und Epitaxie maßgeblich zum hohen Entwicklungsstand dieser Disziplinen in Deutschland und damit zu zahlreichen technischen und wirtschaftlichen Erfolgen beigetragen. Durch die kontinuierliche Optimierung der Kristallstrukturanalyse konnten immer wieder neue Einsatzgebiete erschlossen werden, z.B. in der Landwirtschaft, in der pharmazeutischen Industrie, im Bauwesen oder in der Textilindustrie.

Für die Entwicklung neuer Materialien spielt die Analyse komplexer Kristallstrukturen eine wichtige Rolle: Erst wenn bekannt ist, welche Struktur zugrunde liegt, können zusätzliche Eigenschaften integriert werden. Bei smarter Kleidung werden z.B. verschiedene physiologische Parameter, wie Körpertemperatur oder Herzfrequenz, über Sensoren erfasst. Je nachdem, wie das Messergebnis ausfällt, können die verarbeiteten Stoffe einen kühlenden oder wärmenden Effekt erzeugen.

Als Gründungsmitglied von BV MatWerk verbindet DGKK und BV MatWerk eine langjährige vertrauensvolle Zusammenarbeit. Beide Institutionen eint das Anliegen, die kontinuierliche interdisziplinäre Zusammenarbeit unter ihren Mitgliedern ebenso wie den wissenschaftlichen Nachwuchs zu fördern, den Austausch mit Politik, Wirtschaft und Gesellschaft zu intensivieren und die Wahrnehmung von Materialwissenschaft und Werkstofftechnik in Politik und Öffentlichkeit positiv zu beeinflussen.

Die BV MatWerk bedankt sich ausdrücklich für das große Engagement der DGKK für Materialwissenschaft und Werkstofftechnik und wünscht ihr im Namen aller Mitglieder eine weiterhin erfolgreiche Zukunft.

Dr. phil. nat. Ursula Eul

Vorstandsvorsitzende der BV MatWerk e. V.

PROGRAMME

WEDNESDAY, 11.03.2020

10:00 – 10:10 **OPENING** ANDREAS DANILEWSKY, ANDREAS ERB

SESSION 1 CHAIR PROF. DR. ANDREAS DANILEWSKY

10:10 – 10:50 **PROF. OLIVIER GUILLON,** FORSCHUNGSZENTRUM JÜLICH GMBH
(INVITED) *Crystalline materials for electrochemical energy storage*

10:50 – 11:10 **DR. DIRK KOK,** RADBOUD UNIVERSITEIT NIJMEGEN, NL
Thermochemical heat storage using alcohol solvates

11:10 – 11:30 **DR-ING. MATTHIAS GERRMANN,** ISABELLENHÜTTE, DILLENBURG
VGF-Growth of Half-Heusler-material for industrial production of thermoelectric-material

11:30 – 11:50 **TOM SCHNEIDER,** TU BERGAKADEMIE FREIBERG
3D interlayer growth in the high temperature vapor phase epitaxy of GaN

11:50 – 12:10 **DR. NIKOLAY ABROSIMOV**, LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG, BERLIN
Growth of ^{28}Si crystals for the preparation of Si spheres

12:10 – 13:20 LUNCHBREAK

SESSION 2 CHAIR PROF. DR. PETER WELLMANN

13:20 – 14:00 **DR. MATTHIAS SCHRECK,** UNIVERSITÄT AUGSBURG
(INVITED) *Single crystal diamond wafers by heteroepitaxy: Synthesis and potential applications*

14:00 – 14:20 **DR. LUTZ KIRSTE,** FRAUNHOFER IAF, FREIBURG
X-Ray Diffraction analysis of the defect structure of diamond substrates and Thick Diamond Films

14:20 – 14:40 **DR. STEPHAN MÜLLER,** FRAUNHOFER IISB, ERLANGEN
PVT growth of large freestanding C-doped AlN crystals

14:40 – 15:00 **DR. THOMAS STRAUBINGER,** LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG, BERLIN
Growth of bulk AlN crystals: Influence of the temperature field on growth rate, optical absorption and dislocation density

15:00 – 16:30 POSTERSESSION WITH DRINKS AND SNACK

SESSION 3 CHAIR PROF. DR. ANDREAS ERB

16:30 – 17:10 **PROF. DR. GÜNTHER EGGELER,** RUHR-UNIVERSITÄT BOCHUM
(INVITED) *On mosaicity and the formation of defects during Bridgman processing of Ni-base single crystal superalloys*

17:10 – 17:30 **TIMMY REIMANN,** INNOVENT E.V, JENA
Magneto-optical Bismuth substituted rare-earth iron garnet sensor films for characterization of electrical steel sheets

17:30 – 17:50 **DARREN PEETS *PhD*,** TECHNISCHE UNIVERSITÄT DRESDEN
Self-flux growth of single crystals of BaCoSO

17:50 – 18:10 **MARIUS PETERS,** GOETHE UNIVERSITÄT FRANKFURT AM MAIN
Crystal growth of the valence fluctuating system $EuPd_2Si_2$

18:30 – 20:30 MITGLIEDERVERSAMMLUNG (GENERAL ASSEMBLY)
WITH DRINKS AND SNACK

THURSDAY, 12.03.2020

SESSION 4 — CHAIR DR. WOLFRAM MILLER

08:30 – 09:10 (INVITED) **PROF. DR. JÖRG NEUGEBAUER,** MAX-PLANCK-INSTITUT FÜR EISENFORSCHUNG, DÜSSELDORF
Modeling crystal growth and materials design in high dimensional chemical and structural configuration spaces

09:10 – 09:30 **DR. NORA WOLFF,** HELMHOLTZ-ZENTRUM BERLIN FÜR MATERIALIEN UND ENERGIE
Growth of $CuFeO_2$ single crystals by the optical floating-zone technique

09:30 – 09:50 **DR. NATALIJA VAN WELL,** LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN
Investigation of orthorhombic and tetragonal phases of $Cs_2CuCl_{4-x}Br_x$ mixed system

09:50 – 10:10 **SEBASTIAN GRUNER,** FRAUNHOFER THM FREIBERG
Investigation of facet growth in heavily doped silicon single crystals grown in the mirror furnace

10:10 – 10:40 COFFEEBREAK

SESSION 5 — CHAIR PROF. DR. MATTHIAS BICKERMANN

10:40 – 11:00 **PROF. DR. MICHAEL HEUKEN,** AIXTRON, SE HERZOGENRATH
Control of AlInN composition in closed coupled showerhead MOCVD reactors

11:00 – 11:20 **DR. ANDREAS POPP,** LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG IKZ, BERLIN
Growth of modulation-doped ß-Ga_2O_3 multilayers by MOVPE

11:20 – 11:40 **DR. CARSTEN DUBS,** INNOVENT E.V, JENA
Nanometer-thin iron garnet films grown by liquid phase epitaxy

11:40 – 12:00 **MANUEL KOLLMUß,** FRIEDRICH-ALEXANDER-UNIVERSITÄT ERLANGEN-NÜRNBERG
Status of 3C-SiC bulk growth using sublimation epitaxy

12:00 – 13:00 LUNCHBREAK

SESSION 6 — CHAIR PROF. DR. MICHAEL HEUKEN

13:00 – 13:40 (INVITED) **DR. ALEXANDER KILLI,** TRUMPF LASER GMBH, SCHRAMBERG
Significance of Optical Crystals for the laser industry

13:40 – 14:00 **PROF. DR. MATTHIAS BICKERMANN,** LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG, BERLIN
Crystal growth of oxides and flourides at the IKZ

14:00 – 14:20 **ANASTASIA UVAROVA,** LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG IKZ, BERLIN
Growth of high-melting sesquioxides for laser applications

14:20 – 14:50 COFFEEBREAK

COMMEMORATIVE EVENT 50 YEARS DGKK A. ERB, W. MILLER, A. DANILEWSKY

14:50 – 15:00 ***OPENING***

15:00 – 15:15 GRUßWORTE - WELCOMING SPEECHES

15:15 – 16:00 GESCHICHTE DER DGKK UND DER ARBEITSGRUPPE “KRISTALLISATION” IN DER VFK
PROF. DR. HELMUT KLAPPER, AACHEN
PROF. DR. PETER RUDOLPH, SCHÖNEFELD

16:00 – 16:20 PRIZES FOR SCHOLAR‘S COMPETITION “WER ZÜCHTET DEN SCHÖNSTEN KRISTALL?“
16:20 – 16:25 POSTER PRIZE

16:25 - 16:50 **DR. ANTON JESCHE,** UNIVERITÄT AUGSBURG
Solution Growth as a powerful tool for the solid-state physicist

16:50 – 17:20 DGKK NACHWUCHSPREIS: **ROBIN LANG**, FRAUNHOFER ISE FREIBURG
MOVPE Growth of GaAs with Growth Rates up to 280 µm/h

17:20 – 17:50 DGKK PREIS: **DR. STACIA KELLER,** UNIVERSITY OF CALIFORNIA ST. BARBARA (USA)
The "amazing" group-III nitrides - epitaxy for optical and electronic applications

19:00 – 22:00 GALA DINNER AT THE MUNICH TOWNHALL (RATSKELLER, ALTE KÜFEREI)

FRIDAY, 13.03.2020

SESSION 7 CHAIR LEV KADINSKI

08:30 – 09:00 **PROF DR. KOICHI KAKIMOTO,** KYUSHU UNIVERSITY, JAPAN
(INVITED) *Collaboration of experiment and numerical analysis of crystal growth of semiconductors*

09:00 – 09:20 **DR. KASPARS DADZIS,** LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG, BERLIN
Model experiments for crystal growth technique

09:20 – 09:40 **STANISLAUS SCHWANKE,** FRAUNHOFER IISB, ERLANGEN
Numerical modeling of metallic impurity incorporation during directional solidification of multi-crystalline silicon assisted by experimental proof

09:40 – 10:00 **OLIVER HARDER,** LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN
Forced convection by high-speed rotation in Czochralski growth from high temperature solutions

10:00 – 10:20 **DR. D.V. BERKOV,** GENERAL NUMERICS RESEARCH LAB. , JENA
Theoretical analysis, critique and validity limits of Haasen-Alexander-Model for predicting the dislocation density

10:20 – 11:00 COFFEEBREAK

SESSION 8 CHAIR DR. JOCHEN FRIEDRICH

11:00 – 11:30 **PROF. DR. STEFAN SCHÖNERT,** TU MÜNCHEN
(INVITED) *High-purity single crystals for experiments in astroparticle physics research*

11:30 – 11:50 **DR. RADHAKRISHNAN SUMATHI** LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG, BERLIN
Towards 80 mm diameter ultra-high purity germanium single crystals by Czochralski growth

11:50 – 12:10 **KEVIN-PETER GRADWOHL,** LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG, BERLIN
Formation of vacancy related defects in high-purity germanium

12:10 – 12:30 **ANGELINA KINAST,** TU MÜNCHEN
$CaWO_4$ crystal growth for the CRESST dark matter search

12:30 – 12:50 **DR. THOMAS JAUß,** ALBERT-LUDWIGS UNIVERSITÄT, FREIBURG
Investigation of particle incorporation in a transparent melt system under µg conditions

12:50 – 13:00 CLOSING REMARKS

POSTERS

1 **MATTHIAS ARZIG**, FRIEDRICH-ALEXANDER-UNIVERSITÄT ERLANGEN-NÜRNBERG
Influence of the surface morphology on the defect distribution in the faceted region of 4H-SiC single crystals

2 **MICHAEL SCHÖLER**, FRIEDRICH-ALEXANDER-UNIVERSITÄT ERLANGEN-NÜRNBERG
Limitations during Vapor Phase Growth of Bulk (100) 3C-SiC Using 3C-SiC-on-SiC Seeding Stacks

3 **MELISSA RODER,** ALBERT LUDWIGS UNIVERSITY FREIBURG
X-Ray Analysis of Defects in 4H-SiC

4 **JOHANNES STEINER,** FRIEDRICH-ALEXANDER-UNIVERSITÄT ERLANGEN-NÜRNBERG
Impact of Varying Parameters on the Temperature Gradients in 100 mm Silicon Carbide Bulk Growth in a Computer Simulation Validated by Experimental Results

5 **DR. KLAUS BÖTTCHER,** LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG, BERLIN
Numerical Modelling of the Czochralski Growth of Neodymium-scandate single crystals

6 **FRANZISKA GRUßLER,** UNIVERSITY OF AUGSBURG
Synthesis and characterization of the triangular antiferromagnets $NaYbO_2$*,* $KYbO_2$ *and* $NaYbS_2$

7 **ELLA SUPIK** ALBERT LUDWIGS UNIVERSITY FREIBURG
The Influence of Sodium Dodecyl Sulfate on the Growth and Properties of Triglycine Sulfate Crystals

8 **ALEXANDER ENGELHARDT,** TECHNISCHE UNIVERSITÄT MÜNCHEN
Single-crystal growth and magnetic phase diagram of $TbFeO_3$

9 **FRANZISKA BREITNER**, UNIVERSITY OF AUGSBURG
Crystal Growth of Fe-doped Li_3N

10 **GLORIA KIRSTE,** LEIBNIZ-INSTITUT FÜR FESTKÖRPER- UND WERKSTOFFFORSCHUNG, DRESDEN
Microstructural evolution of intermetallics under the influence of magnetic field annealing – exemplified by Mn_3Ga

11 **PATRIZIA FRITSCH,** LEIBNIZ-INSTITUT FÜR FESTKÖRPER- UND WERKSTOFFFORSCHUNG, DRESDEN
ZF NMR as a tool to clarify crystallographic, magnetic, and electronic structure of magnetically ordered materials

12 **DR. KRISTIN KLIEMT,** GOETHE-UNIVERSITÄT FRANKFURT
$LnMn_2Ge_2$ (Ln = Nd, Sm, Dy): Single crystal growth and characterization

13 **DR. MATTHIAS SCHUSTER,** FRIEDRICH-ALEXANDER-UNIVERSITÄT ERLANGEN-NÜRNBERG
Directly analyzing the depth dependent properties of $Cu(In,Ga)(S,Se)_2$ wedges manufactured by exfoliation and a nontoxic, adjustable etching process

14 **JIAONA ZOU,** MATERIALS RESEARCH CENTER FMF, FREIBURG
Crystal growth of (Cd,Zn)Te under microgfravity Vampir-F: Characterization of ground experiments

15 **ANDREAS-GABRIEL SCHNEIDER,** UNIVERSITY OF AUGSBURG
In-situ detection of crystallization processes and seed selection in high temperature solutions

16 **DR. WOLFRAM MILLER,** LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG, BERLIN
A KMC model for homoepitaxial growth of Ga_2O_3

17 **JAN PHILLIP WÖHRLE**, ALBERT-LUDWIGS-UNIVERSITY FREIBURG
Investigation of soluto-capillary convection in Ge_xSi_{1-x} melts

18 **IRYNA BUCHOVSKA,** LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG, BERLIN
Parameter study on n-type multicrystalline ingots with tailored resistivity profiles

19 **DR. FRANK M. KIESSLING**, LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG, BERLIN
Investigation of directionally solidified quasi-mono silicon for future gravitational- wave detector test-mass mirrors

20 **STEFAN PÜSCHEL,** LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN
Single crystal growth of Sn- and Ge-substituted $GaPd_2$ for basic research in catalysis

21 **DR. HANS-JOACHIM ROST**, LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG, BERLIN
Thermally stimulated dislocation generation in silicon crystals grown by the Floating Zone method

Invited Talks

CRYSTALLINE MATERIALS FOR ELECTROCHEMICAL ENERGY STORAGE

O. Guillon [abc]

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[b] Jülich-Aachen Research Alliance, JARA-Energy
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Summary

Electrochemical battery cells can be operated reversibly (in charging/discharging modes) in order to temporarily store electrical energy. Among the already commercially available battery systems, the Li-ion technology has been continuously further developed since its discovery acknowledge in 2019 by the Nobel Prize in Chemistry. Reaching high energy densities, Li-ion batteries have enabled new applications in consumable electronics, power tools, battery electric vehicles or even electric flight. Current and future developments focus on the use of new electrode materials, solid-state electrolytes for higher safety and capacity, as well as alternative chemistries such as Na-ion.

Inorganic crystals and polycrystals play a key role in all these type of cells [1]. On the one hand, compounds which can reversibly accommodate mobile Li- or Na-ions in their lattice are used as electrode materials. Today commercial cathode materials for Li-ion batteries are all oxide particles with well-defined stoichiometry and structure. On the other hand, crystalline ionic conductors with negligible electronic conductivity are potentially candidates for solid-state batteries. Their larger electrochemical stability may enable to combine a high-capacity metallic anode with high-voltage cathode materials.

The presentation will give an overview of recent developments in the field and highlight the importance of controlling composition, crystalline phase, morphology and microstructure of crystalline materials by advanced synthesis and processing as well as characterization methods.

[1] Y. Arinicheva, M. Wolff, S. Lobe, C.Dellen, D. Fattakhova-Rohlfing, O. Guillon, D. Böhm, F. Zoller, R. Schmuch, J. Li, Martin Winter, E. Adamczyk, V. Pralong, Ceramics for electrochemical storage, in "Advanced Ceramics for Energy Conversion and Storage", Ed. O. Guillon, Elsevier, 2020.

Single crystal diamond wafers by heteroepitaxy: Synthesis and potential applications

M. Schreck,[a] S. Gsell,[b] M. Fischer[b]

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Summary

Diamond is a crystalline material with a unique combination of extreme material parameters that form the base for various potential applications in mechanics, optics and electronics. Since the 1950s two alternative routes for the synthesis have been explored: The first one is the high pressure high temperature (HPHT) method which copies the natural formation process using typical pressures of 5 - 6 GPa and temperatures of 1300 - 1600 °C. The second one is chemical vapor deposition (CVD) that works at conditions below ambient pressure (10 - 300 mbar) and at more moderate temperatures (500 – 1200°C). While the HPHT technique can deliver crystals of high structural quality, it suffers from severe limitations in size (< 1 inch). In contrast, CVD methods can readily be scaled to large lateral dimensions. However, CVD grown films are typically polycrystalline which hinders their use for high end applications like electronic devices. To tackle this dilemma, heteroepitaxy of diamond on foreign single crystals has been explored. The success of this approach was recently documented by the first report of a 3.5 inch size single crystal diamond wafer (s. Fig. 1).

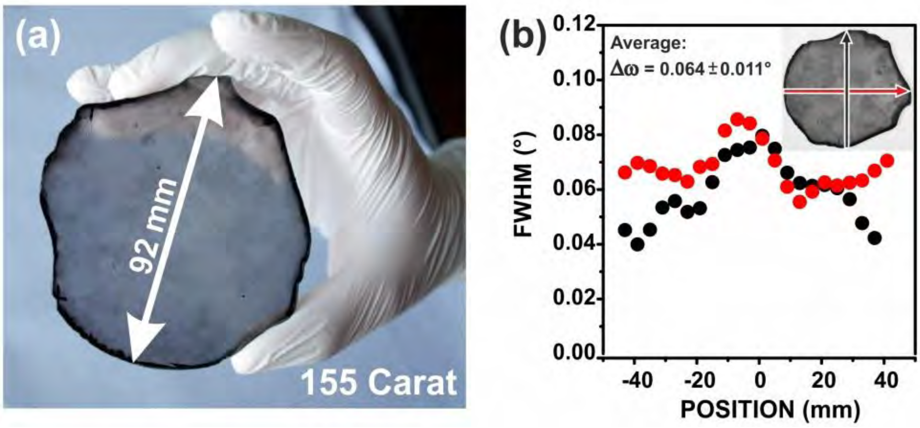

Fig. 1: (a) Free-standing single crystal diamond wafer grown heteroepitaxially on Ir/YSZ/Si(001). (b) Width of rocking curve measured along two perpendicular lines across the wafer. The corresponding average azimuthal width (dia(311) reflection) was 0.12±0.04° and the Raman line width 1.75±0.07 cm^{-1} [1].

In this presentation the efforts towards the realization of single crystal diamond in wafer-size will be reviewed. Important milestones, like the selection of iridium as growth surface, the use of the bias enhanced nucleation (BEN) procedure to generate oriented nuclei, the transformation of highly oriented diamond layers into real single crystals, the development of the multilayer substrate Ir/YSZ/Si and its scaling to wafer-size are described. Special attention is paid to threading dislocations, their role in stress formation and strategies to reduce their density. The state of the art in terms of structural quality for (001)- and (111)-oriented layers is presented and the potential for further improvement is critically discussed. In addition, the model explaining the non-classical diamond nucleation on Ir by the BEN procedure will be briefly outlined [1].

The second part is focused on the material properties relevant for different applications. These comprise

1) detectors for high energy particles at accelerator facilities [2]
2) Schottky barrier diodes [3]
3) monochromators for neutrons [3]
4) host material for color centers as single photon emitters and quantum sensors [4]
5) UV-VIS and IR optical components
6) cutting tools for high precision machining of optical quality surfaces
7) scalpels for eye surgery

While some applications are already in a mature stage with first products being available on the market (http://www.audiatec.de), for others strong further efforts will be required, e.g. to develop high power electronic devices that can compete with alternative wide bandgap semiconductor materials.

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On mosaicity and the formation of defects during Bridgman processing of Ni-base single crystal superalloys

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Summary

Ni-base single crystal superalloys (SX) are used to make blades for turbines which operate in aero engines and power plants and have to withstand mechanical loads at temperatures close to the melting point of the complex alloys. The materials are produced following an ingot metallurgy processing route, where melts are directionally solidified using a Bridgman process. Directional solidification is the first step in a processing chain, where specific heat treatments follow to establish the final microstructure. However, the dendritic solidification of the metallic melt is the first process which coins the SX microstructure, Figure 1 [1].

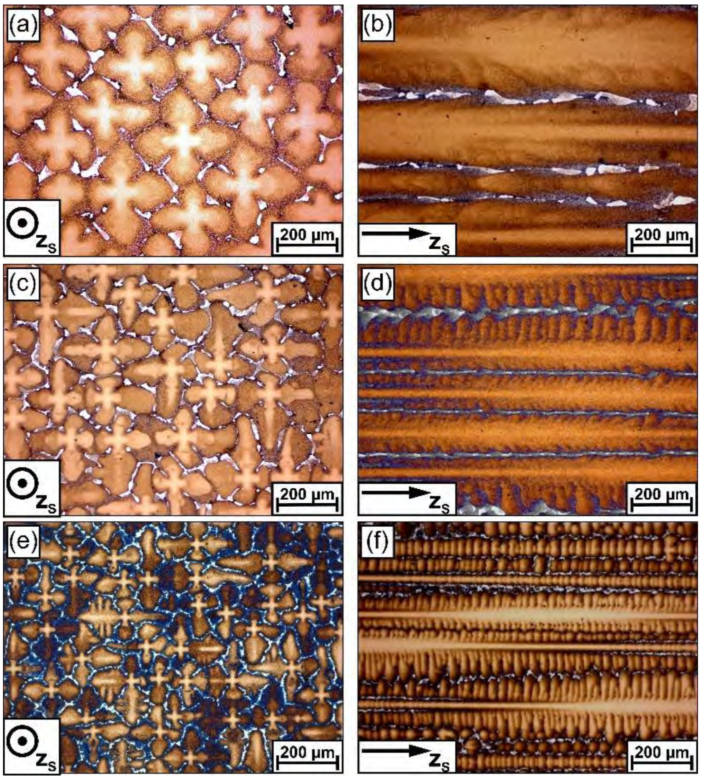

Fig. 1: Dendritic microstructures after Bridgman processing of SX. (a), (c) and (e): Metallographic cross sections perpendicular to the solidification direction. (b), (d) and (f): Longitudinal cross sections. Soldification rates: Top - 45 mm/h; Middle - 180 mm/h; Bottom 720 mm/h.

The Ruhr-University Bochum and the Friedrich-Alexander University Erlangen Nürnberg have joined forces in the collaborative research center SFB/TR 103, which focusses on basic aspects which help to design a new generation of SX. In this context, elementary processes which occur during single crystalline solidification and which lead to the formation of crystal defects require careful attention. With this in mind, a seeded Bridgman process was developed which allows to produce cylindrical crystals of 12 mm diameter and 120 mm. Nucleation and competitive growth of dendrites is investigated using optical scanning electron microscopy.

In order to characterize misorientations between dendrites, a new orientation imaging SEM technique was developed, which allows to document and quantify crystal mosaicity at a high angular resolution [2]. In the present work we describe our seeded Bridgman procedure. We describe the elementary microstructural processes which we have identified. Finally, we present our new orientation imaging SEM method, which has an angular resolution < 0.03°.

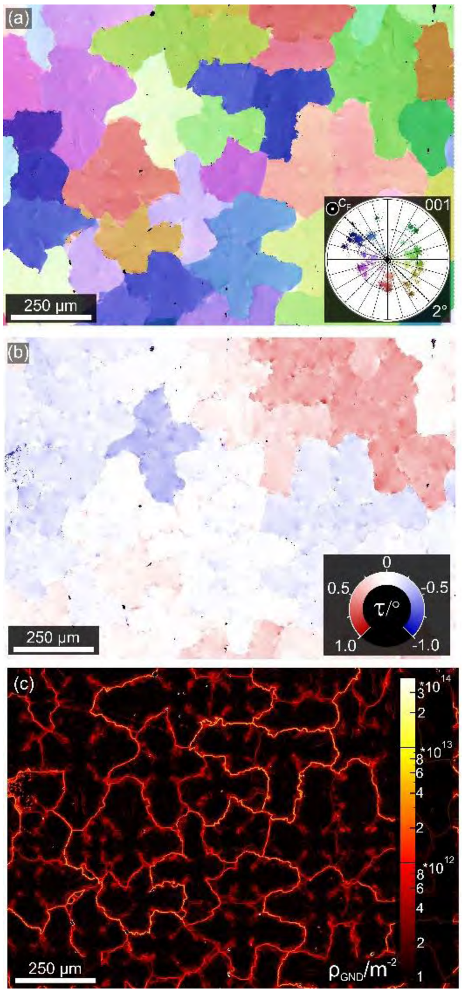

Fig. 2: Results obtained with the new orientation imaging scanning electron microscopy method (the rotation vector base line method, RV-EBSD method) [2]. (a) Out of plane misorientations due to bending processes. (b) Torsional misorientations. (c) Interpretation of misorienations in terms of geometrically necessary dislocations.

The results of the present work are discussed in the light of results which were previously published in the literature. Areas in need of further work are outlined.

Acknowledgement
The authors acknowledge funding through projects A2 and B7 of the collaborative research center SFB/Tr 103 funded by the German research association DFG

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Modeling crystal growth and materials design in high dimensional chemical and structural configuration spaces

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Modern engineering materials have evolved from chemically and structurally simple alloys with well-established design rules to chemically, thermodynamically and structurally highly complex materials. This complexity presents a severe challenge to designing this new generation of materials, since experimental trial-and-error approaches, as successfully used in the past, are often no longer feasible. Ab initio approaches with their inherent predictive accuracy provide perfect tools to explore and identify design strategies, but face serious challenges to efficiently handle the vast high-dimensional configuration spaces resulting from this complexity. To address this challenge, we have developed a python based framework called pyiron that combines (i) rapid prototyping of the complex simulation protocols as needed to achieve computational efficiency and accuracy, (ii) a seamless integration to big data analytics and machine learning tools, as well as (iii) a simple upscaling from interactive prototyping to high-throughput calculations on supercomputer frameworks. The flexibility and the predictive power of this approach will be discussed for examples covering various aspects of crystal growth and materials design.

SIGNIFICANCE OF OPTICAL CRYSTALS FOR THE LASER INDUSTRY

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Summary

TRUMPF Laser is a leading manufacturer of high-power laser systems for industrial applications. The product portfolio of solid-state lasers ranges from high power CW lasers used for welding and cutting applications, to pulsed lasers used in micro machining applications [1].

In this presentation the significance of high-quality optical crystals is shown for a variety of use cases in industrial high-power laser systems.

The first presented use-case is the optical isolator, which is a system critical component for high power pulsed laser systems such as short pulsed and ultrafast lasers [2].

The second use-case is the electro-optical modulator that can be deployed in cavity dumped resonators and regenerative amplifiers. TRUMPF offers a range of kW-class ns lasers based on the principle of cavity dumping [3]. On the other hand, the well-established product line TruMicro 5000 uses regenerative amplification and in our case an electrooptical modulator [4]. On the very high-performance range of regenerative amplifiers TRUMPF offers the “Dira”, a high energy (100s of mJ) high power (up to kW range) ultrafast laser that can be used for various scientific applications such as a drive laser for OPCPA [5, 6].

The third use-case is the conversion of infrared laser radiation into the visible spectral range and ultraviolet regime using nonlinear optical crystals. Many industrial micromachining processes are unthinkable without frequency conversion of CW, short pulse and ultrafast lasers. A prominent example is the lift-off of flexible displays from their mother glass [7], another one the welding of copper using a green CW laser [8].

Acknowledgment
The author thanks the EU and the BMBF for various grants that enabled research projects in the forefront of product development.

[1]https://www.trumpf.com/en_INT/products/lasers/
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[3]https://www.trumpf.com/en_INT/products/lasers/short-and-ultrashort-pulse-laser/trumicro-series-7000/
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Collaboration of experiment and numerical analysis of crystal growth of semiconductors

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Summary

Silicon (Si) and wide bandgap crystals are one of the main materials for solar cells, power devices and/or large scale integrated circuits. For the present power devices, Si crystals grown by the floating zone method are used so far [1]. To satisfy the demand for solar cells and electric vehicles in society, a huge amount of cells and electric power equipment is required; thus, driving demand for Si crystals used in power devices. To satisfy the large demand, it is necessary to grow Si crystals by the Czochralski (CZ) method, and it is particularly essential to concentrate on the carrier's long lifetime in the crystal. Several papers have reported the increased lifetime, and it has been reported that the lifetime of the Si crystals grown by the CZ process is affected by oxygen and/or carbon-related defects [2, 3].
Many papers have reported the carbon impurity in crystals and the formation of oxygen-related defects, such as oxygen precipitates, thermal donors, and new thermal donors [4, 5]. Several papers have also reported that the concentration of carbon in the crystals depends on the process parameters, such as total pressure and flow rate of argon (Ar) gas in a furnace [3, 6]. However, no research has been conducted to measure the level of carbon monoxide (CO) during the Si crystal growth.
We focused on in-situ measurement of CO gas concentration after the melting process of raw materials in the CZ growth method to qualitatively understand the CO contamination mechanism into the Si melt in this paper. We succeeded in to measure the CO concentration in the furnace after the melting process, which is the most crucial process in which CO gas could contaminate the Si melt [6, 7]. The contamination process was then observed and discussed using a simple mass transfer model. Although the results obtained by numerical simulation were reported [8-10] the experimental results have not been reported quantitatively.
We carried out in-situ measurements of CO concentration in a CZ furnace using a gas chromatographic method. Two sampling monitors were set up above the Si melt and the Ar gas exhaust, respectively. The gas samples were collected into the tubes at the two sampling monitors, then introduced to an analyzer made by GL Science. The sampling interval was set at 660 seconds. The melt was made with 25 kg of commercially available polycrystalline silicon in a quartz crucible 45.7 cm in diameter. CO was mainly generated by a heater which caused a chemical reaction at high temperature. In this case, we measured the concentration after melting process without growing crystal.
Figure 1 shows the total pressure dependence of CO concentrations in the furnace measured. The cross indicates the values obtained from the experiment without the Si melt and the quartz crucible. The CO concentration linearly increased as the total pressure in the furnace increased. The value was well above one order of magnitude smaller than that with the Si melt and the crucible. The two measurements linearly increased with one order of magnitude difference. Both values of measured CO concentration proportionally increased with the total pressure in the furnace.
The average velocity of Ar gas decreased as a function of the total pressure based on the ideal gas law. Therefore, as the gas velocity in the furnace declined, back diffusion of CO was enhanced. Consequently, the CO concentration increased as a function of the total pressure in the furnace. As

CO flowed from the heater to the exhaust, the CO concentration at position A near the exhaust increased.

Figure 2 shows the measured CO concentrations as a function of the total flow rate of Ar gas in the furnace. As the total flow rate of Ar gas increased, the CO concentration decreased. The significant decrease in CO concentration as a function of gas flow rate was due to the higher Péclet number (the ratio between the convective and the diffusive mass transfer of Ar gas flow).

The increase in gas flow could also remove more SiO from the system, which was the reactant of the CO generation. Such decrease in CO contamination was attributed to the increase of flow velocity as well as the effective removal of SiO from the chemically reactive area in the furnace.

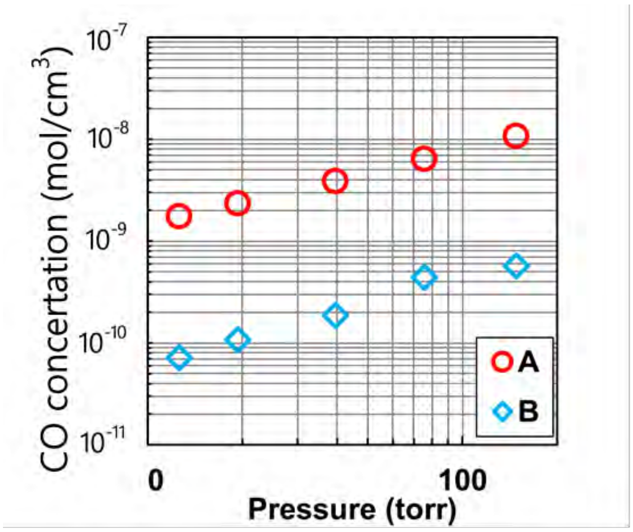

Fig. 1: Measured CO concentration as a function of Ar gas pressure in the furnace.

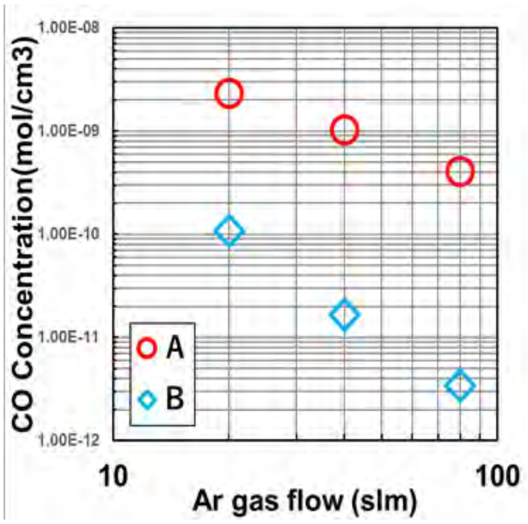

Fig. 2 Measured CO concentration as *a function of Ar gas flow rate.*

Acknowledgment

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High-purity single-crystals for astroparticle physics research

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Summary

The dynamics of galaxies, larger structures, and the overall expansion and structure formation in the universe require about six times more gravitating mass than can be ascribed to ordinary matter. As this type of matter is invisible, it is called dark matter (DM). It probably consists of a hitherto undetected type of weakly interacting elementary particle and is searched for in many experiments around the globe. DM particles with masses from sub-GeV to the TeV would occasionally hit nuclei in the laboratory and the small recoil energies in the tens-of-keV range can be identified in direct detection experiments using high-purity single crystals. High-purity $CaWO_4$ crystals are operated in the CRESST dark matter experiment [1] at a few tens of mK temperature, where it serves as target material for the interaction with dark matter particles. Energy thresholds below 100 eV for nuclear recoils have been achieved and the average background rate measured with $CaWO_4$ crystals grown at TUM [2] corresponds to about 3.51 kg−1 keV−1 d−1 in the energy region between 1-40 keV [3], which is significantly lower compared to crystals of the same material with different origin.

High-purity crystals are also employed to address another fundamental question in particle physics, astrophysics and cosmology, namely why matter is so much more abundant than anti-matter in today's Universe. The question might be closely related to the observation that neutrino masses are more than five orders of magnitude smaller than that of the electron. This raises the question whether the origin of neutrino masses differs from that of the other elementary fermions. The leading models on neutrino masses, rooted in unified field theories, predict that neutrinos are their own antiparticles, usually referred to as Majorana neutrinos. Given that they do not carry electrical charge, neutrinos are the only known elementary fermions where the strict distinction between particle and antiparticle could be void. Majorana neutrinos would not only explain naturally the lightness of neutrinos, but would also shed light on the mechanism why matter is so much more abundant than anti-matter in today's Universe. Majorana neutrinos lead to a nuclear decay which violates lepton number conservation and is therefore forbidden in the standard model of particle physics. The so called neutrinoless double beta decay transforms in a nucleus with mass number A and atomic number Z, two neutrons simultaneously into two protons, under the emission of two electrons, 2e-, but without the emission of two electron anti-neutrinos. The two electrons carry the available decay energy and the resulting mono-energetic signal is the prime experimental signature. A positive detection would manifest the first observation of a matter-creating process, without the balancing emission of antimatter. The GERDA experiment at the Gran Sasso underground laboratory is operating background-free [4] high-purity germanium single crystals, enriched in the isotope ^{76}Ge. A world leading median sensitivity of the half-life of $T_{1/2} > 1.1 \cdot 10^{26}$ yr (90% C.L.) has been reached recently [5].

This presentation will discuss the science motivations, the state-of-the-art and the future the needs for high-purity crystals in astroparticle physics experiments of the current and next generation.

Acknowledgment
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Acknowledgment

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