Polish Conference on Crystal Growth

June 19th-24th, 2022

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Dear participants,

It is with the greatest pleasure that we host you in Gdańsk for a conference aimed at exchanging knowledge and experience in the theoretical and experimental aspects of crystal growth and its applications.

The PCCG 2022 conference is the fourteenth in a series of international meetings organized by the Polish Society for Crystal Growth. The event is co-organized by the Gdańsk University of Technology, the Polish Society for Crystal Growth and the ENSEMBLE3 Center of Excellence.

We wish you successful discussions, finding answers to your nagging questions, and establishing fruitful scientific cooperation. We wish you a good time in Gdańsk and we hope that you leave here with the best possible memories.

Thank you for joining us!

Tomasz Klimczuk

/Chair of the Organizing Committee/

Michał Leszczyński

/Chair of the Scientific Committee/

Plenary talks

P-1 *Monday 20.06.2022,9:00-9:35*

Epitaxial Topological Insulator Heterostructures

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Topological insulators (TIs) of the Bi(Sb)-chalcogenide class of materials exhibit a complex lattice structure, consisting of $Bi(Sb)_2Te_3$ quintuple layers adjoined to each other by weak van der Waals forces. As a result, a layered crystal structure is formed that determines the physical properties as well as epitaxial growth. Moreover, the “openness” of the lattice structures provides a variety different lattice sites for incorporation of doping elements used to tune electronic or magnetic properties of the materials. In this presentation, the properties of growth by molecular beam epitaxy as well as the peculiar structural and electronic properties are described.

Particular focus will be on the magnetic doping used to induce magnetism in TI materials [1]. Ferromagnetism leads to the opening of a magnetic band gap in the topological surface state of TIs that enables the realization of the quantum anomalous Hall effect due to formation of dissipation less edge channels without external magnetic fields. However, doping of the Bi-chalcogenide TIs with transition metal elements such as manganese leads to a pronounced structural modification of the material due to the formation of natural self-assembled heterostructures that consist of quintuple layers alternating with septuple layers such as with $MnBi_2Te_4$ in a large variety of different stacking sequences [2]. Detailed structure analyses reveal that the magnetic doping atoms are indeed concentrated within the septuple layers with different degrees of disorder. This strongly enhances the magnetic exchange interactions which increases the magnetic Curie temperatures as well as the magnetic band gap of the Dirac electrons [2,3], which is a key parameter for achieving the anomalous quantum Hall effect at higher temperatures. Apart from these “natural” heterostructures, MBE allows to directly grow artificial TI heterostructures comprising of different TI and normal insulator layers. We present here the striking example of TI/NI heterostructures based on the IV-VI lead-tin chalcogenides, in which the quantization of Dirac states can be effectively tuned and controlled as shown by theory and experiments [4]. This opens up the means for band gap engineering as in traditional semiconductor heterostructures.

** Collaborators: S. Wimmer, A. Ney, G. Krizmann, H. Hajlaoui, H. Groiss, G. Bauer, M. Hoffman, A. Ernst (JKU Linz), O. Caha, J. Michalička, J. Ruzicka,V. Holy (CEITEC/Univ. Brno), J. Sánchez-Barriga, E. Rienks, P. Mandal, E. Schierle, F. Freyse, E. Weschke, O. Rader (BESSY II, Berlin), P. Küppers, M. Liebmann, M. Morgenstern (RWTH Aachen), V. Volobuiev, R. Rechciński, M. Galicka, P. Kacman, R. Buczko (IFPAN, Warzawa), R. M. Otrokov, E. V. Chulkov (San Sebastian), M. Albu, G. Kothleitner (FELMI Graz), D. Primetzhofer (Univ. Uppsala), G. Bihlmayer (FZ Jülich), S. A. Khan, J. Minar (Univ. Pilzen), H. Ebert (LMU München),*

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Crystal growth and spin triplet superconductivity in UTe_2

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UTe_2 attracts much attention because of the spin-triplet supercondudctivity and unusual properties[1]. It crystallizes in the body-centered orthorhombic structure with the space group, Immm (#71, D_{2h}^{25}). The large Sommerfeld coefficients (γ=120 mJ $K^{-2}mol^{-1}$) manifests a heavy electronic state. Superconductivity occurs at 1.5-2 K in the paramagnetic ground state. One of the highlights in UTe2 is the huge upper critical field, H_{c2}. Figure 1 shows the H_{c2} curve of UTe_2 when the field is applied along the *b*-axis. Field-reentrant superconductivity appears above 15 T, and superconductivity survives up to the metamagnetic field, H_m=35 T, which highly exeeds the Pauli limit. For H || *a* and *c*-axes, H_{c2} also exceeds the Pauli limit. Thus the spin-triplet state is naively expected. A microscopic evidence for the spin-triplet state is indeed obtained from the Knight shift in NMR experiments. At the moment of discovery of superconductivity, UTe_2 had been thought to be at the verge of ferromagnetic order with strong ferromagnetic fluctuations. Figures 1 shows the comparisons with the field-reentrant (or reinforced) H_{c2} curves in URhGe and UCoGe, in which ferromagnetism and superconductivity coexist. The reentrant behaviors are mainly due to the field induced ferromagnetic fluctuations when the field is applied along the hard magnetization axis. In UTe_2, ferromagnetic fluctuations are, however, not confirmed experimentaly, alternatively antiferromagnetic fluctuations with the incommensurate q-vector are detected in the inelastic neutron scattering experiments. In UTe_2, both antiferromagnetic and ferromagnetic fluctuations as well as valence, and Fermi surface instabilities may play important roles for superconductivity. Another important highlight in UTe_2 is the multiple superconducting phases under pressure and the field-induced phenomena, which also support a spin-triplet scenario because of the spin and orbital degree of freedom. In this talk, we present our recent progress on UTe2, focusing on the high quality single crystal growth and superconducting properties.

This work was done in collaboration with G. Knebel, D. Braithwaite, A. Pourret, J. P. Brison, Q. Niu, M. Valiska, G. Lapertot, S. Raymond, J. Flouquet, D.X. Li, F. Honda, A. Nakamura, Y. Shimizu, Y. Homma, Y. J. Sato, M. Kimata, A. Miyake, C. Paulsen, W. Knafo, I. Sheikin, H. Harima, Y. Yanase, Y. Haga, H. Sakai, K. Ishida

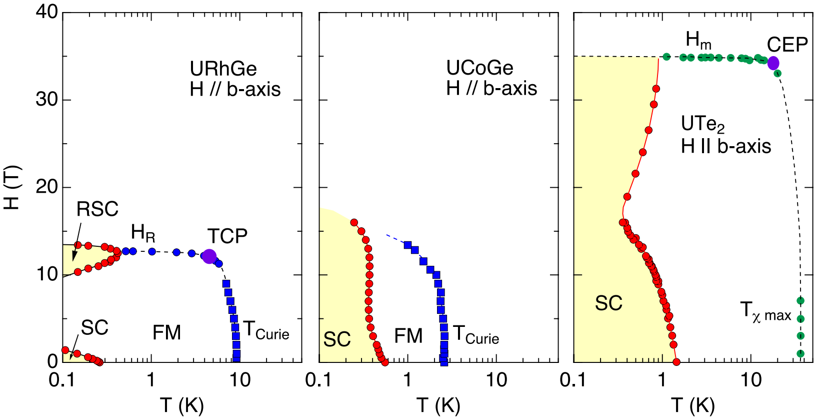

Fig.1 H_{c2} curves in ferromagnetic superconductors (URhGe, UCoGe) and UTe_2

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P-3 *Monday 20.06.2022, 14:00-14:40*

$(\mathrm{LaSe})_{1.14}(\mathrm{NbSe}_2)_{m=1,2}$ crystals a lot alike NbSe_2 single layer but heavily doped

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Transition metal dichalcogenides including NbSe_2 host a rich variety of exciting physical ground states as superconductivity and charge density waves. Those can be affected by doping using electrical field transistor effect or deposition of K atoms but as we have shown in [1] a significantly stronger doping is introduced in the misfit layer single crystal of $(\mathrm{LaSe})_{1.14}(\mathrm{NbSe}_2)_{m=2}$ where LaSe layer dopes two adjacent NbSe_2 with 0.57 electrons per Nb atom. Then, the system band structure is a NbSe_2 monolayer alike but rigidly shifted by 0.3 eV.

It is known that NbSe_2 monolayer with broken in-plane inversion symmetry and strong spin-orbit coupling features the Ising superconducting pairing [2] protected by spin-momentum locking with an in-plane cririical magnetic field $B_{c2//ab}$ strongly violating the Pauli limit B_P. It is a very 2D effect since upon increasing the number of NbSe_2 atomic layers $B_{c2//ab}$ becomes rapidly smaller than B_P. Recently, we have shown [3] that bulk $(\mathrm{LaSe})_{1.14}(\mathrm{NbSe}_2)_{m=2}$ with $T_c = 5.7$ K displays extremely high $B_{c2//ab} = 50$ T and $(\mathrm{LaSe})_{1.14}(\mathrm{NbSe}_2)_{m=1}$ is a recorder holder with $T_c = 1.23$ K and $B_{c2//ab}$ more than 20 T, which is 10 times more than B_P beating a NbSe_2 monolayer. Interestingly, if the same chemical model applies in $(\mathrm{LaSe})_{1.14}(\mathrm{NbSe}_2)_{m=1}$ as in $(\mathrm{LaSe})_{1.14}(\mathrm{NbSe}_2)_{m=2}$, a charge transfer of 1.14 electron per NbSe_2 unit is expected. However, this is impossible since the undoped NbSe_2 unit can accept at most one electron. This indicates that the NbSe_2 band could be completely filled, while the metallicity/superconductivity would reside in LaSe layers. Our recent transport, STM QPI and ARPES experiments and DFT calculations however show [4] that although the doping of NbSe_2 is significanly higher than in case of $(\mathrm{LaSe})_{1.14}(\mathrm{NbSe}_2)_{m=2}$ it is less than 1.14 electron. Then, the resulting bandstructure is still monolayer NbSe_2 alike with the Fermi level very close to the top of the hole band. We discuss La vacancies as a reason of the reduced charge transfer, here. Also, the reason why the Ising coupling survives in our 3D crystals consisting of alternating insulating LaSe and (super)conducting NbSe_2 atomic layers will be addressed.

This work was supported by the projects APVV-20-0425, VEGA 1/0743/19, and IMPULZ IM-2021-42

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Integrated Crystal Growth of Advanced Nanomaterials: from model systems to integrated manufacturing

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Motivated by the many new device concepts and unique opportunities that 1D and 2D nanomaterials enable to drive nascent technologies such energy efficient ICT [1,2], we systematically adapt in-operando metrology to "unblind" their crystal growth processes and to accelerate their development cycles as scalable industrial materials particularly via chemical vapour deposition (CVD) based process technology. Using in-operando transmission electron microscopy we could reveal the key processes of catalytic group IV and III-V nanowire growth [3], allowing for instance the switching between zinc-blende and wurzite structure with atomic precision [4]. Using in-operando scanning electron microscopy and X-ray photoelectron spectroscopy, we could expand insights from catalytic graphene CVD [5] to nucleation and growth dynamics of compound mono-layer crystals such as h-BN and WS_2 [6,7]. The talk will highlight the interdisciplinarity this comprises, ranging from metallurgy and new approaches to epitaxial metal growth [8] to defect characterization by multi-dimensional super-resolution microscopy [9] and machine-learning assisted materials discovery.

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P-5 *Tuesday 21.06.2022, 9:35-10:10*

Ga(Al)N diluted with arsenic: Epitaxial growth by MBE and MOVPE, novel structural properties and functionalities

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Following the breakthrough of group-III nitrides in short wavelength optoelectronics cubic GaAsw diluted with nitrogen was intensively studies for infrared emitters. Less attention has been paid to wurtzite GaN diluted with group-V lelements like As, P, Sb and Bi. Most important results will be summarized [1].

The growth of nitrogen-rich GaNAs by MBE was performed and studied by XPS, XRD, SEM, TEM, SIMS and PL. Strong shifts of the valence band could be confirmed [2]. Under metal-rich conditions As acts as antisurfactant and novel GaN microrods were grown characterized by dodecagonal walls with stable a- and m-planes (fig.1) [3]. The rod growth is of VLS-type with native Ga-droplets forming the caps. The electrochemical properties are not well studied so far and possible applications for water splitting will be presented.

Whereas by MBE only up to 0.6% As could be incorporated into Ga(Al)N with MOVPE up to 5% As incorporation was conformed by XRD measurements. By MOVPE as growth methods flat wurtzite layers of hiogh crystallinity can be grown. Results on the As incorporation into AlGaN will be presented as well.

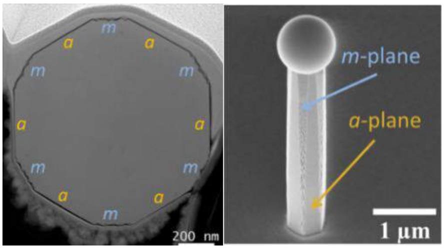

Fig.1 STEM-HAADF of a horizontal cross section and SEM image showing rough and smooth sidewalls [3].

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Exploration of metastable perovskite-type transition-metal oxides : High pressure synthesis and computational approach

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Searching for an exotic quantum phase in a simple system is an attractive and challenging task in condensed matter physics. Perovskite-type transition-metal oxides have been widely studied as a typical platform with high chemical controllability suitable for such task. So far, we have focused on perovskite oxides with unusually high-valence transition-metal ions such as Fe^{4+}, Co^{4+}, and Cu^{3+}. Whereas they show anomalous magnetic and electronic properties reflecting the strong p-d hybridization, their comprehensive characterization has been hampered by the difficulty of high-pressure synthesis.

In this talk, I will introduce our recent progress on the high-pressure synthesis and computational approach for perovskite-type oxides with unususually high-valence metal ions, which exhibit exotic magnetic phases as topological helimagnetic states and possible spin-liquid-like states. A simple cubic perovskite $SrFeO_3$ is found to show a rich variety of helical spin structures involving quadruple-q topological helimagnetic state hosting a hedgehog spin texture [1]. To further explore novel phases potentially coupled with charge degrees of freedom, we established phase diagrams of $Sr_{1-x}La_xFeO_3$ [2] and $(Sr_{1-x}Ba_x)_{2/3}La_{1/3}FeO_3$ [3], and found the spin-charge fluctuation inherent to the phase competition between the G-type antiferromagnetic phase and spin-charge ordered phase. As another example exhibiting spin spirals, we show cubic perovskites $Sr_{1-x}Ba_xCoO_3$ [4] and orthorhombic perovskites $Sr_{1-x}Ca_xCoO_3$ [5,6] and discuss their magnetism in terms of double-exchange interactions mediated by itinerant oxygen p-holes [7].

For the second half of my talk, I will present a novel orthorhombic perovskite cuprate $PrCuO_3$ with quasi-one-dimensional chains of CuO_4 with square-planar coordination [8]. The structural analyses suggest that the formation of the Cu-O chain is caused by the AB site charge transfer and the cooperative Jahn-Teller distortion of nearly divalent Cu ions. Upon the La substitution for Pr, we found the abrupt change in structure and electrical conductivity, which is accompanied by the AB site charge transfer. From magnetization and heat capacity measurements, a possible emergence of a quantum spin-liquid state will be discussed. Finally, I show computational structure predictions by convex hull calculations with density functional theory and Bayesian optimization for oxygen-deficient perovskite-type cuprates [9] and A-site ordered perovskite-type ferrites [10].

This work was done in collaboration with M. Onose, H. Takahashi, T. Osaka, H. Sakai, Y. Yamasaki, H. Sagayama, T. Nakajima, J.-H. Kim, D.S. Inosov, B. Keimer, Y. Tokura, and A. Seko. This work is supported in part by KAKENHI (Grants No. 17H06137 and 22H00343), Murata Science Foundation, and Asahi Glass Foundation.

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P-7 *Wednesday 22.06.2022, 9:35-10:10*

(Cd,Mn)Te as a material for X and gamma ray detectors. Technology and physical properties

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In recent years, a series of investigation has been devoted to a possibility of using crystals based on CdTe with addition of manganese for X and gamma ray detectors.

The aim of our studies was to check whether the (Cd,Mn)Te crystals may be easily obtained by the Low Pressure Bridgman (LPB) method in the form of large, homogeneous, very high resistivity single crystals with as few as possible twins, subgrains, and tellurium inclusions. The elements used: Cd, Te and Mn were of the highest purity available at the moment.

The first critical parameter is the $\mu_e \cdot \tau_e$ product, where μ_e is the carrier mobility (here electrons) and τ_e is the carrier lifetime (here also electrons).

The second parameter is a value of the resistivity ρ, which should be (as a result of compensation) of the order of ~1010 Ω·cm.

For characterization of the (Cd, Mn)Te samples we used optical, electrical, $\mu_e \cdot \tau_e$, and ρ mapping measurements. Photocurrent–Voltage (PC-V) measurements were compared with the room-temperature Am-241 gamma-ray response current. Our result show that the measurements of the Photocurrent (PC) kinetics are sensitive to the quality of the sample surface, and may be used as a tool to test methods of preparation of detector plates.

This work was supported by the Polish National Centre for Research and Development through grant No. TECHMATSTRATEG1/346720/8/NCBR/2017.

Topological and quantum materials: from crystal growth to applications in photonics

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Topological and quantum materials open new perspectives to the field of photonics, thanks to their rich electronic band structure that enables outstanding optical properties intertwined with quantum phenomena [1]. Here, we correlate the electronic, optical and quantum properties of such materials, and show how they are and can be harnessed to develop novel photonic devices. A special emphasis is made on interband plasmonic and giant refractive index properties, topological surface states, quantum confinement, dynamic tuning of the electronic, optical and spin properties, in materials such as topological insulators and semi-metals. The approaches to produce and structure such materials are discussed. The discussion includes the growth of macroscopic crystals, top-down structuring, and bottom-up self-assembly, and shows how these approaches can be combined to obtain functional microstructures, nanostructures, or metamaterials.

The authors acknowledge support from the ENSEMBLE3 Project (The Centre of ExcelleNce for nanophotonicS, advancEd Materials and novel crystal growth-Based technoLogiEs) which is carried out within the International Research Agendas Programme (IRAP) of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund.

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Formation of nitride semiconductor nanowires by plasma-assisted molecular beam epitaxy

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Group-III nitride nanowires (NWs) are promising alternative to planar heterostructures exhibiting significant potential to drive new applications especially when integrated on low-cost platforms. Due to easy elastic relaxation of lattice strain, NWs are of high crystallographic perfection even when grown on lattice-mismatched or non-crystalline substrates. As the result, highly lattice-mismatched NW heterostructures can be obtained defect-free, which is crucial in many applications, including nanoscale electronics, optoelectronics, and biochemical sensing devices.

In this talk the mechanisms active during plasma-assisted molecular beam epitaxy (PAMBE) growth of group-III nitride NWs will be reviewed. We will start from the very basic presentation of PAMBE GaN growth modes and then move to description of processes taking place at various stages of NW formation. In particular, we will show an important role of *in-situ* growth monitoring (by laser reflectometry, reflection high-energy electron diffraction and line-of-sight quadrupole mass spectrometry) for understanding and quantifying those processes. Then, an influence of a substrate and its surface uniformity on self-induced nucleation and growth as well as on properties of GaN NWs on non-crystalline substrates will be discussed. Specifically, their impact on NW arrangement on the substrate and mixed polarity of the NWs inside the ensemble will be shown. Finally, some future trends in development of PAMBE growth technology of NW-based device structures will be briefly presented.

Financial support from the Polish National Science Centre (grant 2016/23/B/ST7/03745) is acknowledged.

Application of high-pressure spectroscopy in the study of semiconductor structures

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High hydrostatic pressure generated in diamond anvil cell (DAC) is an efficient experimental tool allowing to obtain a lot of data which are difficult or not possible to get by other methods. In particular, it can be used to verify mechanisms of light emission in semiconductor structures.
An overview will be given on the high-pressure studies of phenomena influencing the radiative transition energy and emission efficiency in nitride (In,Al,Ga)N and oxide (Zn,Mg)O alloys and heterostructures [1,2,3]. They include:

- carrier localization processes and the presence of localized donor states,
- conduction band filling and non-parabolicity effects,
- effects related to built-in electric fields being a consequence of a spontaneous polarization caused by asymmetry of atomic bonds in materials with a wurtzite structure, and piezoelectric polarization generated in quantum structures due to lattice mismatch, observed in both nitride and oxide structures grown in polar directions.

Also, the results of high-pressure studies of ZnO and ZnMgO epitaxial layers will be presented, showing a significant influence of strain on their optical properties and phase transition pressures.

Acknowledgements: This work was partly supported by the National Science Centre, Poland, by grant number 2012/05/B/ST3/03113.

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Biological Mineralization of Hydrophilic Intraocular Lenses

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Biomaterials calcify upon implantation in order to replace malfunctioning tissues, when they are in contact with biological fluids, which are supersaturated with respect to more than one crystalline phase of calcium phosphate. The implantation of intraocular lenses (IOLs) for cataract treatment has been hailed as a major advance. Hydrophilic acrylic IOLs, made of Poly(2-hydroxyethyl methacrylate) (PHEMA), despite other advantages which made them popular among surgeons, upon contact with aqueous humor, exhibit significant incidence of opacification which is due to the formation of calcium phosphate crystals, mainly hydroxyapatite ($Ca_5(PO_4)_3OH$, HAP). The aqueous humor is supersaturated with respect to HAP. Calcification, takes place on the surface and in the interior of the IOLs. Clinical findings were duplicated by laboratory experiments through the development of appropriate experimental models. In batch reactors, the kinetics of IOLs was measured and the mechanism was investigated at conditions of constant driving force, i.e. supersaturation. It was found that the formation of HAP was surface diffusion controlled. Crystallization of calcium phosphates on the surface of the IOLs was preceded by long induction times inversely proportional to the supersaturated solution. Surface hydroxyl ionized groups are suggested to favor the local development of high supersaturation by surface complexation. Polar carbonyl groups of the acrylic polymer may also play a similar role. Long contact time of the IOLs with aqueous humor resulted in the formation of calcium phosphate in the interior of the IOLs by the diffusion of the calcium and phosphate ions inside the polymeric matrix.

Epitaxial Growth development of (100) β-Ga_2O_3 by MOVPE

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Our modern society relies on a wide range of electrical and electronic systems, which require the conversion of primary electricity into another form of electricity. Therefore, the conversion of electrical energy must be carried out as efficient as possible. To fulfill this goal ultra-wide bandgap semiconductors are necessary. One high potential candidate regarding the application field of power transistors is beta-gallium oxide (β-Ga_2O_3) which owns a bandgap of ≈ 4.8 eV. Due to this high band gap a high breakdown field strength of up to 8 MV/cm results. Transistors based on this material will be able to switch high voltages with less power losses and significantly smaller drift regions - the basis for more compact systems.

In this report, we will present the challenging path of the homoepitaxial growth development of β-Ga_2O_3 thin films by metal organic vapor phase epitaxy (MOVPE), to obtain β-Ga_2O_3 structures tailored for high power devices. As substrates (100) oriented Mg-doped (semi-insulating, for horizontal device architecture) and Si-doped (conducting, for vertical device architecture) wafers prepared from bulk crystals [1], also developed in-house at IKZ, have been used. First, we will discuss the formation of twin lamellae in epi-layers on the semi-insulating substrates and how to avoid them by applying vicinal surfaces through an accurate miscut of the substrates. Next, we will focus on the development of high quality layers as the base material for lateral devices [2]. A full control of the desired growth mode (step-flow growth) was obtained by adjustment of the growth parameters, in particular gallium to oxygen ratio to the substrate miscut [3]. However, to achieve the best exploitation of the breakdown field a vertical architecture for β-Ga_2O_3 based transistors is necessary. Therefore, the final step of the film growth development includes challenges defined by vertical device architecture, which are quite different from the lateral case. Here, layers with low doping (10^{16} cm^{-3} range) concentrations and layer thicknesses of several micrometers, while maintaining a low density of structural and point defects, are crucial [4]. Thick layers require, therefore, an increase of the growth rate. The concluded growth process enabled us to prepare high quality structures suitable for power devices in both horizontal and vertical configurations, with outstanding electrical properties.

This work was performed in the framework of GraFOx, a Leibniz ScienceCampus and funded by the BMBF under Grant Nos. 03VP03712 and 16 ES1084K, the European Community [Europäische Fonds für regionale Entwicklung (EFRE)] under Grant No. 1.8/15, and the Deutsche Forschungsgemeinschaft under Project Funding Reference No PO-2659/1-2.

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Invited talks

Macrosteps dynamics and the growth of crystals and epitaxial layers

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Step pattern stability of the vicinal surfaces during growth was analyzed using various surface kinetic models. It was shown that standard analysis of the vicinal surfaces provides no indication on the possible step coalescence and therefore could not be used to elucidate macrostep creation during growth. A scenario of the instability, leading go macrostep creation was based on the dynamics of the step train. The critical is step motion at the rear of the train which leads to double and multiple step creation. The condition is that the step density ratio in and out of the train lower than 2 prevents double step formation irrespective of the kinetics. For higher step density ratio low density of the step promotes single step stability. Fast step kinetics from lower terrace stabilizes the single steps slow (high barrier) is promoting step coalescence. The incorporation kinetics from upper terrace role is close to neutral. The creation of double step creates slow the step in front to accelerate and catch the previous double step while those behind catch up the double step creating multistep structure. The multistep are not mobile as the alimentation leads to emission of single step which moves forward. The final structure consist of macrosteps and superterraces with the number of single steps moving forward. Thus the single step motion is essential crystal growth mode despite the presence of the macrosteps. The macrostep are prone to creation of the overhangs which results from surface dynamics coupling to impingement from the mother phase. The angular preferential access of the bulk material to the macrostep edge, leads to diffusive instability. Therefore it is expected that harmful influence of the macrosteps by creation of inclusions and dislocation is stronger during growth from the liquid phase [1] .

The research was partially supported by National Science Centre, Poland grants number 2016/23/B/ST5/02278 and 2021/41/B/ST5/02764.

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I-2 *Monday 20.06.2022, 11:00-11:25*

Various aspects of strain relaxation in InGaN epilayers

Julita Smalc-Koziorowska[1,*], Joanna Moneta[1], Ewa Grzanka[1], Marcin Kryśko[1], Grzegorz Muzioł[1], Marcin Siekacz[1], Grzegorz Targowski[1], Czesław Skierbiszewski[1], Tobias Schulz[2], Martin Albrecht[2]

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Epitaxy of high In-content $In_xGa_{(1-x)}N$ layer is needed for realization of nitride based optoelectronic devices emitting light in green or red range of waveleghts or to produce $In_xGa_{(1-x)}N$ based solar cells. One of the problem in the epitaxy of high In-content $In_xGa_{(1-x)}N$ layers is limitation of the In content in coherently grown layers to around 30% which is related to a high lattice mismatch between InN and GaN of 11%. Strain relaxation of $In_xGa_{(1-x)}N$ layers is important in respect of realization of higher lattice constant substrates for epitaxy of high In content $In_xGa_{(1-x)}N$ based structures. We studied the various aspects of the strain relaxation mechanism of $In_{0.2}Ga_{0.8}N$ deposited on various substrates and grown by molecular beam epitaxy or by metal-organic vapour phase epitaxy. The mismatch stress of the layers may be relieved by introduction of (a+c) misfit dislocations via slip on pyramidal {1122} planes [1], inclination of threading dislocations coming from the substrate or the newly generated ones, or by elastic relaxation at V-pits. Plan-view TEM and cathodoluminescence studies of misfit (a+c) dislocations showed the 3° rotation from the $\langle 1\bar{1}00\rangle$ directions, which are the expected propagation directions of these dislocations in the basal (0001) plane. The reason for the rotation may be related to dissociation of the dislocation core and cross-glide of the partial dislocations to other pyramidal $\{1\bar{1}01\}$ planes.

The introduction of misfit dislocations by slip on pyramidal planes requires high activation energy and is delayed for layers, where other mechanisms are activated first. Consequently, the $In_{0.2}Ga_{0.8}N$ layers deposited on sapphire exhibit lower state of strain relaxation in comparison to identical layers deposited on bulk GaN crystals (Fig.1).

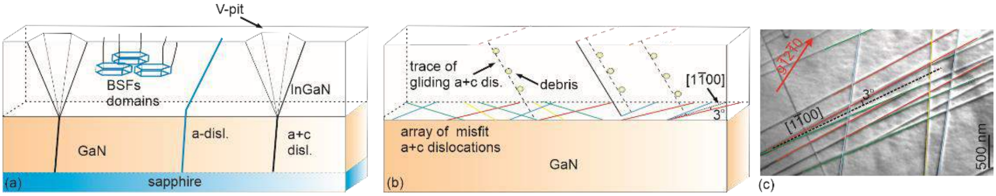

Fig.1 (a) and (b) schemes of the relaxation mechanisms of In0.2Ga0.8N layer deposited on (a) GaN/sapphire template or on (b) bulk GaN substrate; (c) plan-view bright field TEM image of the In0.2Ga0.8N layer deposited on bulk GaN substrate.

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Ga vacancies in MOVPE prepared GaN layers – correlation with other point defects

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Defects related to gallium vacancies (V_{Ga}) are extremely important for optoelectronic applications since they are believed to be a cause for non-radiative recombination of carriers [1]. By other authors, it is believed that V_{Ga} are responsible for yellow band luminescence and form non-radiative centers if they are in complex with donors [2-4]. V_{Ga} related defects deteriorate the frequency properties of high electron mobility transistors (HEMT) since trapping and releasing charge in deep levels is rather slow process decreasing the cut off frequency. V also enhance migration of atoms and can cause quantum well decomposition or decrease the device lifetime.

Set of GaN layers prepared by MOVPE under different technological conditions were investigated by Variable energy positron annihilation spectroscopy (VEPAS). The aim was to find a link between technological conditions, GaN layer properties and V_{Ga} formation. VEPAS is unique and irreplaceable method to get information about V_{Ga} concentration in thin epitaxial layers. Different correlations between technological parameters and V_{Ga} formation were observed for layers grown from TEGa and TMGa precursors. In case of TEGa formation of V_{Ga} was significantly influenced by type of reactor atmosphere (N_2 or H_2), while no similar behaviour was observed for growth from TMGa. Formation of V_{Ga} was suppressed with increasing temperature for the growth from TEGa. On the contrary, enhancement of V_{Ga} formation was observed for growth from TMGa with cluster formation for the highest temperature of 1100°C. From the correlation of PL results with calculated V_{Ga} concentration it can be concluded, that increased V_{Ga} concentration enhances excitonic luminescence. Probable explanation is that V_{Ga} prevents formation of some other highly efficient nonradiative defect. Anticorrelation between V_{Ga} formation and carbon contamination was observed.

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Growth and engineering of two-dimensional crystals: from Xenes to transition metal dichalcogenides

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Nowadays, the class of two-dimensional (2D) crystals encompasses a large variety of members including synthetic single-element materials, referred as Xenes[1], and multi-element layered crystals, like transition metal dichalcogenides (TMDs).[2]

The Xene family quickly expanded in the last ten years: after a first generation developed starting from the elements of the IV column of the periodic table (e.g., silicene, germanene, and stanene), a second one emerged with the elements of the adjacent columns (e.g., borophene, antimonene, tellurene, etc.).[1] Here, we report on epitaxy of silicene, stanene, and their heterostructure,[3] discussing also the case of blue-phosphorene. We focus on the epitaxial methodologies and configurational details aiming at the identification of the key points for nanotechnology, e.g. scalability, quality, and stability aspects.

Concerning the TMDs family, we overview our recent advances in the growth of atomically thin layers of molybdenum disulfide (MoS_2) and ditelluride ($MoTe_2$) carried out by chemical vapour deposition (CVD) approaches. We explore both the chalcogenation of pre-deposited metal precursors and the pure vapor phase reaction of precursors aiming at controlling homogeneity, quality, and thickness (down to the single layer limit) of the deposited TMDs.[4,5] We show that the use of perylene-based seeding promoters is beneficial for the formation of the layers in the 2D form, even at the extreme asperities of patterned substrates where the interfacial surface adhesion of the layers competes in a delicate balance among strain and slip-and-shear mechanisms. Moreover, we show that finite element method calculations allow us to predict the concentration gradients and carrier gas fluxes governing the CVD processes for the optimization of the deposition conditions and the control of the allotropic phase of the deposited TMDs.

Both for Xenes and TMDs, artificial shape modifications, combining strain engineering and spatial anisotropy, are presented as a strategy to expand the pool of 2D materials technological applications.[5]

Acknowledgement: funding from H2020 ERC-COG grant n. 772261 "XFab".

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Van der Waals epitaxy - challenges and opportunities

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Recent research activity focused on transition metal dichalcogenides (TMD) layered materials, enabling acquiring extremely thin flakes via exfoliation from bulk crystals, brought attention of the research community to possibilities of epitaxial growth of TMDs. Even though the exfoliated TMD flakes are suitable for research purposes, they are not much useful for application-ready optoelectronic devices, since it is not possible to control their shapes and dimensions. That's why the epitaxial growth techniques came into play. Due to the layered nature of TMDs with a plane of transition metal (TM) atoms confined in-between two planes of chalcogen atoms, there are no unsaturated dangling bonds at the TMD surfaces. In the bulk the subsequent TM-chalcogen-TM trilayers are bound only by the Van der Waals forces. The same applies in the case of TMD deposited on any substrate and in this context the Van der Waals epitaxy is an accurate expression describing such situation. In spite of the weak bonds between the TMD layer and the substrate usually the layer has a distinct orientation with respect to the substrate, but in contrast to the conventional epitaxy the lattice matching between TMD layer and the substrate is not importnat, only the symmetries of both lattices should be similar.

I will show two examples of TMDs – $MoTe_2$ and $NiTe_2$ grown by molecular beam epitaxy on GaAs(111) substrates, and an example of TM pnictide (TaAs) grown on GaAs(001). TMDs grow on GaAs in a proper Van der Waals epitaxy mode. The case of TaAs can be described as a pseudo Van der Waals epitaxy, since the structure of this material is closed to but not completely layered. All three above mentioned materials are topological semimetals. $MoTe_2$ in one of its polytypes is a Weyl semimetal (WSM), $NiTe_2$ is a Dirac semimetal (DSM), and TaAs is a WSM. Since the electrical properties of topological semimetals are to very much extent dependent on a magnetic field, the possibility of the epitaxial growth of DSM and WSM opens a way of integrating them in heterostructures with ferromagnets and antiferromagnets and get use of magnetic proximity effects. The in-plane lattice parameters of two above-mentioned materials ($MoTe_2$ and TaAs) are close to 3.4Å, not matching any common substrate for epitaxy, and have about 20% lattice mismatch to GaAs. In this context the Van der Waals epitaxy is important. The lattice matching of $NiTe_2$ to GaAs(111) is much better (lattice mismatch of about 3%) but here also the Van der Waals epitaxy growth mode is valid.

This work has been supported by the Polish National Science Centre (NCN) through the project No. 2017/27/B/ST5/02284

I-6 *Tuesday 21.06.2022, 10:10-10:35*

Structural and electronic heterogeneities of boron-doped diamond nanoarchitectures

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The work is focussed on the heterogeneous structural and electronic behaviour of various boron-doped materials extending from zero-dimensional particles through polycrystalline or nanostructured three-dimensional surfaces. A boron-doped diamond reveals large heterogeneities induced by numerous factors, inter alia multi-faceted crystallinity, inhomogeneous boron concentration, sp^2/sp^3-carbon ratio, surface terminations and grain size distribution. The single nanodiamond particles and a nanostructured diamond, which are fabricated by either a top-down or a bottom-up procedure. Nanoarchitectured surfaces allow high areas and large aspect ratios to be achieved, exhibiting highly heterogeneous charge-transfer performance for catalytic, sensing and energy applications. We have anticipated multi-factor-originated heterogeneities tuned by geometric, physicochemical and electronic properties of diamond displaying the essential fabrication and diagnostic methodologies and critically reviewing their benefits and drawbacks. The current CVD and HPHT technologies have been developed and improved since the early 90s and their capabilities are practically exhausted in terms of hardware available on the market. A good chance of achieving a breakthrough in this area will be the development of a new technology or a significantly modified machine delivering homogeneous power to the growth surface over large areas (i.e. scaling a linear antenna system or DC arc plasma jet CVD).

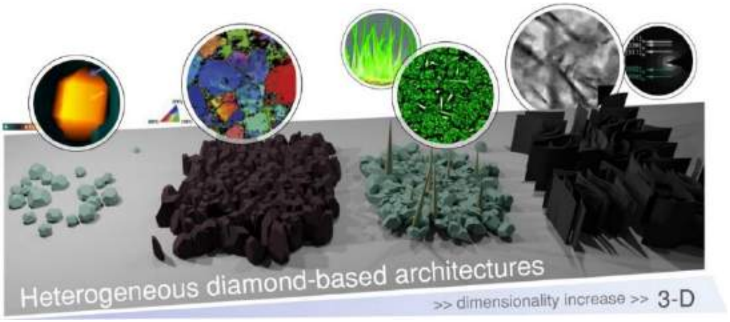

Fig.1 Multi-dimensional diamond-built architectures revealing heterogeneous structural and electronic behaviour.

This research work is supported by the Foundation for Polish Science under grant no. POIR.04.04.00-00-1644/18

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I-7 *Tuesday 21.06.2022, 11:00-11:25*

Perovskite photovoltaic technology on flexible substrates

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Metal halide perovskites constitute a very attractive class of materials foroptoelectronic applications, such as solar cells, light emitting diodes, lasers and photodetectors. Most notably, solid-state photovoltaic devices based on these materials have reached power conversion efficiencies (PCEs) exceeding 25% within only a decade of academic research. Perovskite solar cells have a great market potential, but there still remain few challenges, which need to be resolved to prove viability of the technology. Some of the well-known issues include material stability. Furthermore, cost-effective, reliable fabrication process capable of delivering highly efficient, large-area perovskite modules is of paramount importance. This talk will outline large versatility of perovskite PV technology, focusing on optoelectronic properties of this class of materials. Flexible perovskite solar cells successfully passing IEC-based accelerated aging tests, including damp heat aging, will be presented. Additionally, special aspect of the perovskite technology – all perovskite tandem PV modules - will be discussed and their scalable fabrication process demonstrated, complemented with a robust encapsulation methodology.

I-8 *Tuesday 21.06.2022, 14:35-15:00*

Flux growth as a preparative method for intermetallic phases

Michał J. Winiarski[1,*], Karolina Górnicka[1], Zuzanna Ryżyńska[1], Igor Oshchapovskyy[1], Leszek Litzbarski[1], Ebube E. Oyeka[2], Thao T. Tran[2], Tomasz Klimczuk[1]

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The metal flux is widely used for the growth of single crystals of various systems, especially intermetallic phases. The simplicity of the method together with its versatility and relatively low costs makes it the tool of choice for synthesizing many complex solid state systems. The popularity of the method among the solid state chemistry and physics community is highlighted by the increasing number of citations of the seminal review papers by Canfield and Fisk [1] and Kanatzidis *et al.* [2].

I will discuss our experience of the growth of several Al-rich ternary intermetallic phases, including $A\mathrm{Co_2Al_9}$ (A = Sr, Ba) – isostructural analogues of "catastrophic CDW" system $\mathrm{BaFo_2Al_9}$ [3,4], complex magnetic systems $R\mathrm{Ni_3Al_9}$ and $R_3\mathrm{Ni_5Al_{19}}$, and the family of cage compounds $R\mathrm{T_2Al_{20}}$ (R – rare earth metals, T = V-Cr) [5]. Most of these systems can be readily synthesized in a polycrystalline form using arc- or induction melting, however Ca-, Yb-, Sm-, and Tm-bearing compounds would, at best, suffer from significant deviations from the nominal stoichiometry due to the evaporation of volatile elements. Moreover, in case of $\mathrm{YNi_3Al_9}$ we found that the detailed structure of the single crystalline form is distinct from the polycrystalline one.

The growth of bismuth-based superconductors $\mathrm{CaBi_2}$ and LiBi [6,7], and a $\mathrm{AlB_2}$-related compound $\mathrm{Yb_2PdGe_3}$ will also be discussed.

I will also address the didactic potential of flux growth experiments of simple binary systems in teaching crystallography and materials science courses.

This research work is supported in part by the Ministry of Science and Higher Education (Poland) under project 0142/DIA/2018/47 ("Diamentowy Grant"), by the National Science Center (Poland) grant (UMO-2018/29/N/ST5/01286), and by the Gdańsk University of Technology AURUM program (project no. DEC-5/2020/IDUB/II.1.3, run within the frame of the Excellence Initiative -Research University.

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I-9 *Wednesday 22.06.2022, 10:10-10:35*

Development of the composite luminescent materials based on the complex oxide compounds using LPE growth method

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The report presents the last achievements of our group at COM IF UKW in the development of the multilayer luminescent materials based on the single crystalline films (SCFs) and single crystals (SCs) of garnets, perovskites and orthosilicate compounds using the liquid-phase epitaxy (LPE) method for application as scintillating materials for radiation monitoring, phosphors for photo-conversion (pc) in white LEDs and photovoltaic cells.

The three mainstreams of the research are considered:

1. Development of multilayer composite scintillators and thermoluminescence (TL) materials based on SCFs and SCs of different oxide compounds for simultaneous registration of different types of ionizing radiation (α-, β-particles and γ-quanta). Such composite scintillators and TL materials have been made in the form of multilayer epitaxial structures containing one or two scintillators in the form of SCFs grown the LPE onto substrates from SC scintillators. The SCs and SCFs parts of CSs have been fabricated from the effective scintillation materials based on the Ce^{3+}, Pr^{3+} or Sc^{3+} doped simple and mixed $A_3B_5O_{12}$ garnets, where A=Lu, Gd, Tb; B= Al, Ga; $(Y,Lu)AlO_3$ perovskites and $(Y,Lu)SiO_5$ orthosilicates with different luminescent spectra and scintillation decay kinetics or different TL glow curves.

The report presents the results on fabrication of composite scintillators and TL materials based on the garnets, perovskites and orthosilicate compounds and the investigation of their scintillation/TL properties. The results of testing of the developed composites in the detectors for radiation monitoring of mixed ionizing fluxes will be presented as well.

2. Development of pc-converters based on SCFs and SCs of simple and mixed garnet compounds for high-power WLEDs. All solid-state pc-converters can be produced in the form of multilayer epitaxial structures containing film converters grown by the LPE method onto substrates from SC converters with different excitation and luminescence spectra. Such types of composite pc-converters have been produced from the efficient luminescent materials on the basis of Ce^{3+} doped mixed garnets with general formula $A_3B_5O_{12}$, where A= Y, Lu, Gd, Tb, B=Al, Ga, grown by the LPE method in SCF form onto undoped and Ce^{3+} doped of YAG, LuAG:Ce and GAGG:Ce garnet substrates.

3. Development of photovoltaic cells based on the doubly layered epitaxial structures $(Y,Gd,Tb)(Ga,Sc)O_{12}:A^{4+},B^{2+}/(Y,Gd,Tb)(Ga,Sc)O_{12}:C^{2+},D^{4+}$ (A=Ce, Pr; B=Ca, Mg; C= Eu, Mn; D=Si, Ge) garnets, grown onto YAG and GGG substrates. These composite structures enable receiving the p-n junctions which can be used for creation of the new generation photovoltaic cells**.** The developed photovoltaic cells in comparison with conventional semi-conductor materials with the band gap <3.5 eV, will be based on the mentioned garnets with energy gap of 6-6.5 eV and the radiation transitions or RE activators arising from the violet range up to the UV one. This allows receiving the p-n junctions which can be used for development of the solar cells using the UV radiation on Earth and cosmic space.

This work was performed in the frame of Polish NCN 2017/25/B/ST8/02932, 2018/31/B/ST8/03390 and 2019/33/B/ST3/00406 projects.

I-10 *Wednesday 22.06.2022, 11:00-11:25*

The surprising chemistry of oxide molecular beam epitaxy

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The materials class of crystalline oxides provides a plethora of functional (dielectric, semiconducting, superconducting, ferroelectric, or ferromagnetic) properties. Molecular beam epitaxy (MBE) is the established method for realizing high quality oxide thin films. In its mostly used variety, the corresponding cation is evaporated from an effusion cell in vacuum onto the heated substrate where it gets oxidized by molecular oxygen, ozone, or an oxygen plasma. The existence of suboxides with significantly higher vapor pressure than their related cation elements leads to a peculiar redox chemistry not only on the growth front but also within the effusion cells. With the example of the plasma-assisted MBE growth of the semiconducting oxides Ga_2O_3, In_2O_3, $(In,Ga)_2O_3$, SnO_2 and its suboxide SnO, I will discuss the implications of this chemistry on growth rate, film composition, and flux emanating from the effusion cells. Three chemical reactions describe the suboxide-related chemistry:
(1.) The reaction of the metal with its oxide towards the suboxide, which is responsible for etching of oxide films [1] but also provides efficient suboxide sources [2].
(2.) The reaction of the cation element with oxygen, which can lead to unintentional suboxide fluxes from elemental sources, leading to unexpectedly high cation incorporation in the grown films [3]. On the growth front, the same reaction provides the p-type oxide SnO [4]. Generally, the suboxide formation on the growth front is the first step during oxide growth. Its thermally activated desorption limit the growth rate.
(3.) The reaction of the suboxide with activated oxygen on the growth front, is the second step that completes oxide growth. A kinetic growth model that involves both these steps, describes the observed, peculiar growth rate dependence on metal-to-oxygen flux ratio and substrate temperature for SnO_2, Ga_2O_3, and In_2O_3 [5]. A simpler, single-step growth kinetics can be realized when the suboxide instead of an elemental cation flux is provided to the growth front, as demonstrated by SnO_2 [2] and Ga_2O_3 [6] films grown by suboxide MBE (S-MBE).
Beyond suboxide kinetics, thermodynamically-driven cation exchange on the growth front, e.g. Ga $\leftrightarrow$ In, leads to the preferential incorporation of Ga over In in $(In,Ga)_2O_3$ films. More importantly, it provides a catalytic growth mechanism, that enables Ga_2O_3 to be grown at higher temperatures and growth rates [7].
Most findings of the presented study can be readily applied to the MBE growth of chalcogenides that possess sub-chalcogenides.

This work was performed within "GraFOx", partially funded by the Leibniz Association.

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Transparent Semiconducting Oxides: bulk single crystals and basic physical properties

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Transparent semiconducting oxides (TSOs) constitute a class of oxide materials combining both semiconducting behaviour and transparency in the visible / UV spectral region. The TSOs drive an extensive research towards novel devices and applications in electronics, opto-electronics, photovoltaics, radiation detection, and gas sensing among others.

In many, if not most of the cases, a device development depends on the availability of bulk single crystals. High melting points (1700 - 2100°C) and thermal instability of the TSOs make the crystal growth directly from the melt difficult and challenging, often requiring novel approaches in crystal growth technology [1]. The TSO compounds to be discussed in terms of bulk crystal growth and basic physical properties include binary (β-Ga_2O_3, In_2O_3, SnO_2, ZnO), ternery ($BaSnO_3$, $ZnSnO_3$, $MgGa_2O_4$, $ZnGa_2O_4$), and quaternary ($Zn_{1-x}Mg_xGa_2O_4$, $InGaZnO_4$) systems. A special attention will be paid to bulk β-Ga_2O_3 single crystals grown by the Czochralski method [2], which attract a particular attention in academia and industry for high-power electronic devices to improve voltage conversion efficiency.

Optical bandgaps of the TSOs in quest range from 2.8 to 5 eV. They are all n-type semiconductors with the free electron concentration ranging from about 5×10^{15} to over 10^{20} cm^{-3}, and electron mobility approaching 300 $cm^2V^{-1}s^{-1}$ [3]. Many of the compounds can also be obtained as electrical semi-insulators. The electrical properties can be tuned in a three-fold manner: by growth conditions, intentional doping, and annealing.

This work was partly performed in the framework of GraFOx, a Leibniz-Science Campus partially funded by the Leibniz Association-Germany; by the Bundesministerium für Bildung und Forschung (BMBF) grants Nos. 03VP03712 and 16 ES1084K; German Research Foundation (DFG) grants Nos. FO 558/3-1, GA 2057/2-1, and GA 2057/4-1, and the Leibniz Senatsausschuss Wettbewerb (SAW) grant BASTET.

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Properties of bare, nitrogen an Al-covered Al and N-terminated AlN polar surfaces determined by density functional theory

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Properties of bare, N- and Al-covered polar AlN(0001) and AlN(000-1) surfaces were determined using density functional theory (DFT) calculations. On Al-terminated AlN(0001) surface at a low nitrogen coverage, Fermi level is pinned by Al broken bond states, located below conduction band minimum. Adsorption of molecular nitrogen is dissociative. In the process electrons are transferred from Al broken bond to topmost N adatom states that depends on the Fermi level. In accordance with electron counting rule (ECR), the DFT results confirm the Fermi level is not pinned at the critical value of nitrogen coverage $\boldsymbol{\theta_N = 1/4\ ML}$, but it is shifted from an Al-broken bond state to Np-z state. For coverage above 1 monolayer (ML), adsorption is molecular. Electronic states of the admolecule are occupied as in the free molecule, i.e. no electron transfer occurs. Accordingly adsorption of the N_2 molecule does not depend on the Fermi level at the surface.

Adsorption of atomic and molecular nitrogen at AlN(000-1) surface was investigated by ab initio calculations and thermodynamic analysis. In equilibrium with Al vapor, the AlN(000-1) surface is thermodynamically stable in two states: under low Al coverage ($\boldsymbol{\theta_{Al} \leq 1/3\ ML}$) and under high Al coverage ($\boldsymbol{\theta_{Al} \approx 1\ ML}$). In these two cases adsorption of nitrogen is completely different. At low Al-covered surface the nitrogen atom is strongly bound to N surface atom, creates the N_2 admolecule that is finally detached creating surface vacancy $V_N(s)$. This energy gain in this reaction is positive. At the fully Al-covered surface atomic nitrogen is adsorbed in T4 sites. Molecular nitrogen dissociates with the energy gain, dependent on additional N coverage. This change is related to the reduction of electron transfer contribution, caused by Fermi level shift down due to electron transfer from Al to N surface states.

On the AlN(0001) surface under Al coverage Al atoms are adsorbed in T4 sites for very low Al coverage, up to $\boldsymbol{\theta_{Al} = 1/3\ ML}$. For higher Al coverage, $\boldsymbol{1/4\ ML \leq \theta_{Al} \leq 1\ ML}$ the adlayer becomes disordered and corrugated vertically. For higher coverage, $\boldsymbol{1\ ML \leq \theta_{Al} \leq 7/6\ ML}$, the Al adlayer becomes ordered and atomically flat. For higher coverage, $\boldsymbol{1.24\ ML < \theta_{Al} < 2\ ML}$, the Al adatoms are located in the second layer with the adsorption energy reduced comparing to the to lower coverage. Thermodynamic analysis identified two regions in equilibrium with Al vapor: first at very low pressures in which $\boldsymbol{\theta_{Al} \leq 10^{-3}\ ML}$ and the second for higher pressures which is $\boldsymbol{1\ ML \leq \theta_{Al} \leq 7/6\ ML}$.

Growth of single crystals of intermetallic compounds from metallic fluxes

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Among the countless number of single crystal growth techniques from the liquid phase, the method high-temperature crystallization from a solution is of particular importance. It consists in dissolving the ingredients at high temperature in a suitable solvent, followed by a slow cooling of the solution, which leads to supersaturation and spontaneous growth of the desired crystals. In the case of preparation of single crystals of intermetallic compounds, the methods of crystallization from metallic fluxes are commonly used. In addition to its undeniable advantages, this technique also has significant disadvantages and limitations.

I present a brief overview of single crystal growth processes for selected pnictides, indides, stannides and germanides prepared to study their basic physical properties. The issues of flux selection, growth procedures and chracterization of the obtained crystals are discussed.

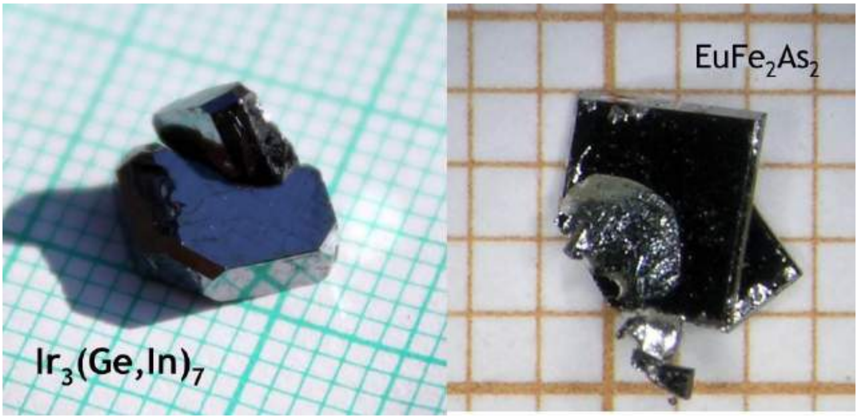

Fig.1 Single crystals of $Ir_3(Ge,In)_7$ and $EuFe_2As_2$.

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Crystal growth and two-phase superconductivity in the locally noncentrosymmetric $CeRh_2As_2$

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The recently discovered $CeRh_2As_2$ has been attracting attention to the unusual two-phase superconductivity [1]. Unique upper critical field (H_{c2}) phase diagrams and a clear thermodynamic phase transition within the superconducting (SC) state demonstrate a low-field even-parity and a high-field odd-parity state. The two-phase superconductivity can be attributed to the centrosymmetric $CaBe_2Ge_2$-type structure of $CeRh_2As_2$ in which the Ce site lacks local inversion symmetry. The local inversion symmetry breaking leads to antisymmetric spin-orbit couplings (ASOC) that allow the same or opposite sign of ASOC for each sublattice degree of freedom. This dictates the superconducting order parameters which are switchable under magnetic fields. We also introduce a crystal growth of some neighboring compounds in the same crystal structure with $CeRh_2As_2$, which imply the crucial role of Ce-4f electrons in the unusual superconductivity [2,3].

In addition to superconductivity, the Ce-4f electron in $CeRh_2As$ plays a versatile role to lead to emergent phases. As-NQR measurements observed a site-selective line broadening below $T_N \sim 0.27$ K, suggesting an antiferromagnetic order that coexists with superconductivity [4,5]. In-depth high-field measurements established rich phase diagrams pointing to the unknown hidden order at $T_0 = 0.4$ K, which is claimed to be the quadrupolar density wave order of the electronic Ce-4f moments [6]. Muon spin relaxation/rotation measurements in various temperatures and magnetic fields characterized anomalous normal-state properties associated with quantum criticality [7].

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I-15 *Thursday 23.06.2022, 14:35-15:00*

Growth and properties of RNiO$_3$ (R = Nd – Lu) single crystals

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RNiO$_3$ perovskites (R - Rare Earth) are a textbook example of strongly correlated oxide system, where interplay between, lattice, charge, and spin degrees of freedom leads to the thermally driven Metal Insulator Transition (MIT) [1]. Temperature of the transition (T_{MIT}) changes gradually with size of R^{3+} ion from 0 K (R = La) to 600 K (R = Lu) [2]. That allows systematic studies of unusual, particularly clean system, which is intrinsically close to the boundary between itinerant and localized behaviour.

Subtle structural distortions and specific charge reordering accompany spontaneous MIT in RNiO$_3$ [3]. Although, the mechanism(s) at the origin of the gap opening in this system is not yet fully understood and has been the subject of lively debate since its discovery in 1991. Moreover, recently observed or theoretically predicted superconductivity [4], unusual non-centrosymmetric antiferromagnetic ordering or multiferroicity [5] have been triggered additional interest by the system.

However, an important drawback for the advancement in the understanding of the complex RNiO$_3$ physics has been lack of single crystals and challenging synthesis procedure, which requires the use of high-pressure and high-temperature.

Here I will present the first ever successful growth of RNiO$_3$ (R = Nd – Lu) bulk single crystals achieved by applying the solvothermal method in temperature gradient under 2000 bar of oxygen pressure [6]. Results of detailed structural and physical properties characterization illustrating excellent quality of obtained crystals will be discussed.

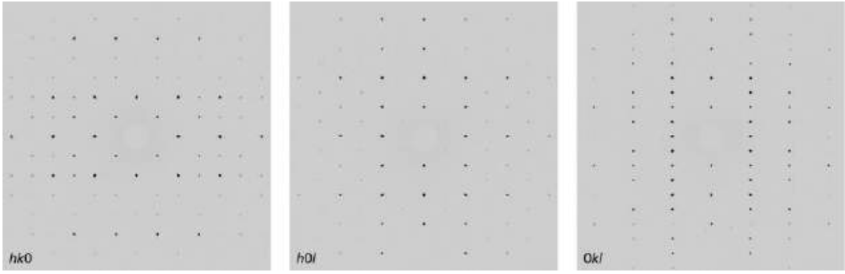

Fig.1 Reciprocal lattice planes of ErNiO3 single crystal (Mo Kα, RT).

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I-16 *Thursday 23.06.2022, 16:00-16:25*

Recent uptaking of All-Solid-State Lithium Battery

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Modern scoeity nowadays cannot escape from the influence of technology. High technology devises play important roles in humanity in many aspects such as daily life, education, health, transporation, *etc*. For example, the more advanced the portable devices are the more they reliable energy storage such as lithium-ion battery and fuel cell.

In this presentation, I talk about three uptaking of energy storage applications as all-solid-state lithium-ion battery. The first is a guideline to sulfide-based solid electrolytes as $Li_7P_3S_{11}$ based on liquid-phase processing [1] (Fig.1a and 1b), and the second is that surprisingly, the mixed solvents [AN+THF+EtOH$_{(one/two\text{-}drop)}$] in the presence of excess sulfide leads to quickly prepare $Li_7P_3S_{11}$ precusor for two mins [2] (Fig.1c). The prepared $Li_7P_3S_{11}$ ehibits ionic conmductivity of 1.2 mS·cm-1 at 25°C. This is higher than that by ball milling and conventional liquid-phase method based on CAN solvent. and futher the third is efficiently liquid-phase synthesis and electrochemical performance of Argyrodite electrolyte Li_6PS_5Cl with highest ionic conductivity *via* chemical factor in the all-solid-state lithium-ion battery [3] (Fig.1d). We proposed the absence of the Li_3PO_4 oxide from Li_6PS_5Cl solid electrolyte could lead to not only increase thse ionic conductivity up to 2.75 mS·cm^{-1} at room temperature (E_a = 24.8 kJ·mol-1) but also significantly increase the stability against the lithium metal after 100 cycles at 0.1 mA·cm^{-2}. Regarding that the Li_3PO_4 impurity from argyrodite could become a serious problem for a battery cell due to the pathway of the Li+ ions being blocked by the impurity, we thus demonstrated that the Li-ion battery cell without Li_3PO_4 in Li_6PSCl argyrodite SE could magnificently increase the capacity of the cell with remarkable stability

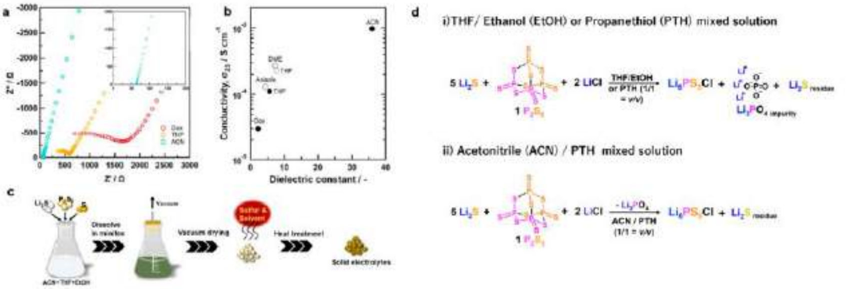

Fig.1. (a) Nyquist plot, (b) inonic conductivity at r.t. for $70Li_2S$-$30P_2S_5$ system, (c) schematics of our novel solution-processing technology for sulfide SEs in this work, and (d) stoichemistry of Li_6PS_5Cl

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Growth of Bulk GaN Crystals

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Along with constantly developing applications of nitride-based devices the demand for native gallium nitride (GaN) wafers is also increasing. In order to fabricate substartes, bulk GaN crystals of the highest structural quality and specified electronic properties have to be grown. Today, three GaN crystallization methods are mainly applied for this purpose: i/ halide vapor phase epitaxy (HVPE) with its derivatives: halide-free VPE and oxide VPE [1-3]; ii/ sodium-flux [4]; and iii/ ammonothermal. The last approach can be basic or acidic depending on what mineralizer is used to increase the solubility of GaN in the feedstock zone [5,6]. This work will cover two of these methods: basic ammonothermal and HVPE.

Properties of amonthermal-GaN (Am-GaN) and HVPE-GaN crystals will be presented. It will be shown that both approaches allow to crystallize material of very high structural quality. The main dopants used to change the conductivity will be shown for both methods.

The main factors limiting crystallization of bulk Am-GaN and novel ways for improving this process will be presented. It will be shown: 1) how to eliminate unwanted lateral growth during crystallization in vertical directions; 2) how the surface of a native seed should be prepared in order to minimize residual stress in the growing crystal; 3) how to obtain uniform and constant supersaturation in the growth zone with many crystals.

In the case of HVPE-GaN growth, the advantages of using native seeds will be demonstrated. The barriers existing for growing truly bulk HVPE-GaN will be analyzed and compared to those in Am-GaN crystallization.

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Influence of structural defects in the $In_{0.3}Ga_{0.7}N$/GaN QWs on their decomposition at elevated temperature

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Although the development of green light emitters technology has been going on for many years, all the time their optical properties differ from blue light emitters. Problem is in structural quality of InGaN/GaN quantum wells (QWs) with high indium content (above 25%) which is needed for green light emission, above 500nm. Low growth temperature, around 700°C, of high indium content QWs has its consequences: (i) directly for QWs: lattice mismatch increase, point defects and impurities density increases, indium fluctuations increases, etc. (ii) indirectly for the growth of quantum barriers, QBs: too low QBs growth temperature favor the formation of trench defects, but too high temperature causes the narrowings in QWs at the upper interface [1]. To avoid or at least reduce the amount of above mentioned defects, special attention should be paid to the proper selection of growth parameters such as V/III ratio, growth rate and pressure. But it happens that some structural defects still remains, and in this work we show how their presence influence on InGaN QWs thermal robustness. It is crucial problem for the design of green light emitting Laser Diode (LD).

Two samples, consisting four QWs, were grown with V/III ratio - 13000. In both cases QWs growth temperature was exactly the same – 700°C. Samples differ in QBs growth temperature: Sample 1T: $T_{QB}=T_{QW}=700^{o}C$, Sample 2T: $T_{QB}=830^{o}C > T_{QW}=700^{o}C$. The basic parameters (HRXRD and PL results) describing such grown QWs are summarized in Table 1.

Table 1

Name	dQWs (nm)	dQBs (nm)	In%	λ (nm)	FWHM (nm)	Intensity	Defects
Sample 1T	2.1	10.8	31	511	32	149	Trench defects
Sample 2T	2	11.9	27	521	35	161	QWs Narrowing

Such prepared samples have been subjected to annealing at elevated temperatures (from 860°C to 920°C) to simulate the growth of p-type layers. Parameters of annealing: 30min, NH_3+H_2 +TEGa atmosphere, reactor Aixtron.

Thanks to detailed HRXRD and STEM analysis it was found that: (i) Sample 1T, with trench defects, starts to decompose at very low temperature – 880°C; (ii) Sample 2T, with narrowings, does not decomposed up to 920°C, Figure 1. Fast decomposition of Sample 1T is associated to the increase of QWs thickness and Indium content inside the trench defect. In the case of Sample 2T, we suspect that it tends to the thickness homogenization during annealing. Thickness homogenization means that average width of the QWs decrease, it significantly increases robustness of the wells. In this work we also show how thermal robustness of the QWs depends on thickness of the QWs and QBs and how it is associated to the point defects (mainly V_{Ga} and V_{In}) diffusion.

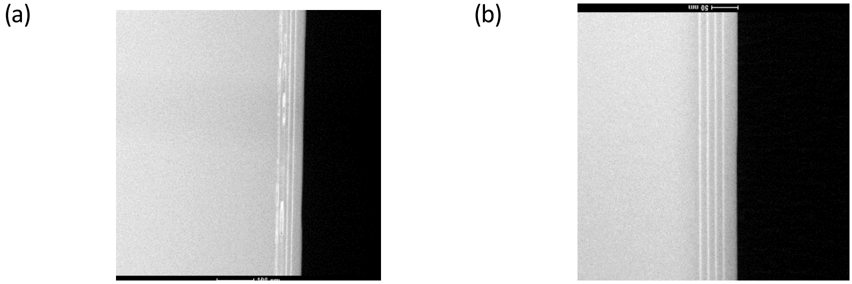

Figure 1: STEM images of (a) Sample 1T and (b) Sample 2T after annealing at temperature 920oC .

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Homogeneous vs. heterogeneous catalyst-free nucleation of GaN nanowires by PAMBE: consequences and opportunities

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A specifically attractive benefit offered by the self-assembled formation of GaN nanowires (NWs) in plasma-assisted molecular beam epitaxy (PAMBE) is the possibility of creating vertically well aligned and single-crystalline NWs even on amorphous layers. Thus the very limited restrictions in terms of the choice of substrate could substantially widen the range of applications based on GaN NWs. However, an in-depth understanding on the self-assembled formation of GaN NWs on non-crystalline layers is still far from being complete. In particular, not much is known about an influence of substrate on GaN NW nucleation.

In this talk the mechanisms of catalyst-free nucleation and PAMBE growth of GaN NWs on amorphous a-Al_xO_y buffer layers will be presented and compared with analogous processes on nitridated Si substrates (SiN_x/Si) that are commonly used for growth of GaN NWs. As will be shown, GaN nucleation on SiN_x/Si is homogeneous and the nucleation rate is limited by surface diffusion and Ga adatom concentration. On the contrary, heterogeneous GaN nucleation is found on a-Al_xO_y buffer layers, so the nucleation rate is determined by density of nucleation centers and Ga capture rate. This leads to enhanced GaN nucleation rate as well as to much wider range of PAMBE growth parameters favoring formation of the NWs on a-Al_xO_y buffer layers as compared to conventional SiN_x/Si substrates. These advantages of a-Al_xO_y nucleation layers are crucial for selective area growth (SAG) of GaN NWs, the topic I will focus on in the second part of the talk. In particular, an important role of Ga adatom surface diffusion for homogeneity of NW lengths in SAG will be discussed. On a general note, our findings demonstrate that nucleation and growth kinetics in SAG depends on the size of the mask pattern, which makes it very different from growth on the equivalent planar layers.

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(grant 2016/23/B/ST7/03745) is acknowledged.

Contributed talks

Carbon in Highly Conductive and Semi-insulating Bulk GaN Crystals

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Halide Vapor Phase Epitaxy (HVPE) is the most common approach for manufacturing gallium nitride (GaN) substrates. The main advantages of this technique are: a relatively high growth rate (>100 µm/h) and the possibility to obtain high-purity material (residual donors and acceptors concentrations are lower than 10^{16} cm^{-3}). Silicon (Si) or iron (Fe), manganese (Mn) and carbon (C) are used as main dopants for crystallizing, respectively, highly conducting (n-type) or semi-insulating (SI) HVPE-GaN crystals [1].

When C substitutes Ga (C_{Ga}) it acts as a deep acceptor and the resistivity of C-doped HVPE-GaN exceeds 10^8 Ωcm at room temperature [2]. A detailed analysis of C in bulk crystals showed that it can be self-compensated [3]. The compensation ratio depends on the C concentration and for its high value (>10^{19} cm^{-3}) the compensation can even reach 1. This means that C, or C-related complexes, can act both as acceptors and donors. Although a lot of research was devoted to C in GaN, a comparison of this dopant in n-type and SI bulk material has not yet been presented. Therefore, in this paper HVPE-GaN crystals co-doped with Si and C as well as Mn and C are studied in detail.

Native ammonothermal seeds of the highest structural quality were used in the HVPE experiments. The morphology, structural quality and growth rate of the co-doped crystals were analyzed applying optical microscopy and X-ray diffraction. Secondary ion mass spectrometry was used to investigate the concentrations of the dopants as well as all the impurities in the crystals. The crystals were also examined in terms of their optical, and electrical properties. For that purpose different characterization methods: Raman spectroscopy, low-temperature photoluminescence and Hall van der Pauw measurements, were applied.

In the HVPE-GaN:Si,C crystals the C concentration was always kept lower than that of Si. The crystallized material was n-type. In the case of HVPE-GaN:Mn,C the concentration of C was higher than that of Mn. The material was semi-insulating at room temperature, but p-type conductivity was revealed in high-temperature measurements.

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C-2 *Monday 20.06.2022, 12:05-12:20*

Structural and optical studies of {ZnO/CdO} superlattices grown by plasma assisted MBE

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The {ZnO/CdO} SL series were grown by plasma-assisted MBE at a different growth temperature of 350-550°C. The ZnO and CdO layer thicknesses were controlled by adjusting the deposition time of the ZnO and CdO sublayers. The structural properties of the SLs were investigated by the high resolution X-ray diffraction (HR-XRD) and the characteristic satellite lines surrounding the main peaks, coming from the periodic structure of SLs, were clearly observed (Fig. 1e and f). X'Pert Epitaxy software based on the dynamical theory of X-ray diffraction was used to simulate the obtained XRD data and to determine the sublayer thicknesses of ZnO and CdO. The growth rate of the sublayers and thus the thickness of CdO and ZnO is growth temperature dependent and correlated with the sticking coefficients of Cd and Zn. Rapid thermal annealing in oxygen flow was applied to study the thermal stability of the SLs. The crystallographic quality of the SLs and diffusion of Cd element were analyzed with TEM (Fig 1a,b,c,d) and seem to depend on the growth temperature. The wurtzite phase of the ZnO sublayers and the rock salt structure of CdO sublayers in the SLs structure were identified. The optical and structural parameters of as-grown and annealed SLs structures significantly change with growth temperature and subsequently annealing.

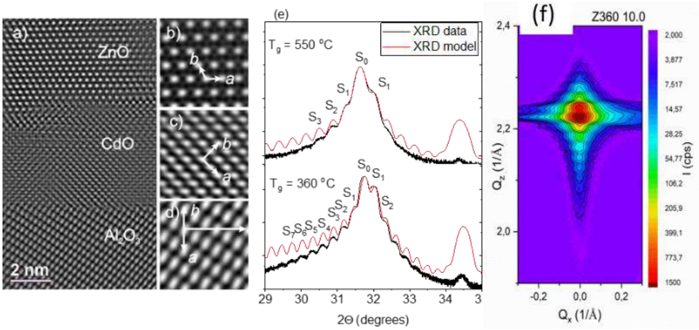

Fig. 1 . (a) HRTEM images of the Al2O3/CdO/ZnO interfaces, (b) enlarged images of the ZnO, (c) CdO, and (d) Al2O3 layers together with the projections of the crystal lattices and translation vectors (e) XRD scans of two SLs structure grown at 360 and 550°C. (f) Reciprocal symmetrical space map of {CdO/ZnO} SLs

The work was supported by the Polish NCN project DEC-2021/41/B/ST5/00216.

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C-3 *Monday 20.06.2022, 12:20-12:35*

Anomalous anisotropy in superconducting of boron-doped diamond growth in rich-deuterium plasma

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The superconductivity in diamond, namely in polycrystalline boron-doped diamond, is one of its most remarkable properties.
In this paper we shows anomalous anisotropy of superconductivity in boron-doped diamond synthesized deuterium-rich plasma. This anisotropy is revealed by R_{XX} and RYY (both in-plane) dependent measurements of the resistive superconducting. Substitute hydrogen by deuterium results in physicochemical differences like enhanced boron doping efficiency [2], rich of (111) phase and lack of degenerative effect on grains which is well-known phenomena [3]. Our diamond films demonstrate the in-plane R_{XX} coherence length significant lover value than in in-plane R_{YY}.

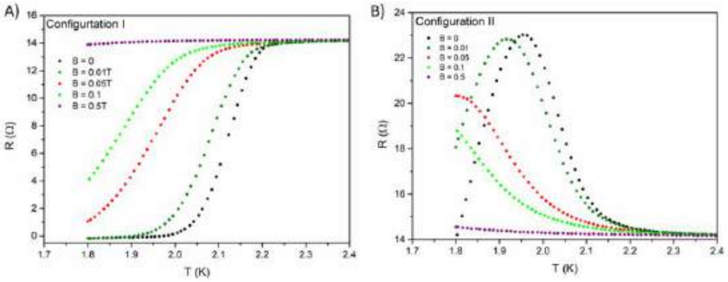

Fig.1 The R(T) of heavily boron-doped polycrystalline diamonds synthesized with the rich-deuterium plasma in MWCVD method, (A) the resistive superconducting transition, (B) the anomalous R(T) peak dimishies with increasing magnetic field.

This superconductivity anomaly can be contributed to bosonic resistive phase transition in disordered diamond arrays.

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Design of High-Temperature Syntheses on the Example of Sn[$PtBi_6I_{12}$]

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In our search for new topological insulators[1], we have discovered new pseudo one-dimensional compounds of heavy elements. The reaction of Bi with Sn, Pt and BiI_3 above 300 °C yielded shiny, black, air insensitive crystals of the subiodide Sn[$PtBi_6I_{12}$] as well as the partially substituted ($Bi_{2x}Sn_{1-3x}$)[$PtBi_6I_{12}$], with $x < 1/3$. Based on extensive studies of the synthetic pathway using differential scanning calorimetry, the two isomorphous compounds could be synthesized independently[2]. Their rhombohedral crystal structures consist of alternating cuboctahedral [$PtBi_6I_{12}$]$^{2-}$ cluster anions and Sn^{2+} or Bi^{3+} cations in octahedral coordination between trigonal faces of two cuboctahedra. These concatenate them into linear chains, making Sn[$PtBi_6I_{12}$] an analogue to Pb[$PtBi_6I_{12}$][3], while ($Bi_{2x}Sn_{1-3x}$)[$PtBi_6I_{12}$], with its vacancies compensating for the higher charge of Bi^{3+}, consists of finite strands, similar to $Bi_{2/3}$[$PtBi_6I_{12}$][4]. The crystals' cube-like morphology originates from six weak Bi···I inter-cluster bridges per cluster connecting the chains. The heavy elements show strong spin-orbit coupling. If this exceeds the width of the chemical band gap of the compound, a non-trivial topology can be expected.

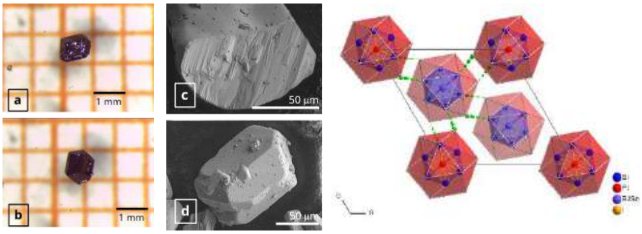

Fig.1 (a, b) Crystals obtained from the optimized synthesis; (c) scanning electron microscopy (SEM) image of a cleaved crystal; (d) SEM image of a crystal; (e) crystal structure projected along the [001] direction with [PtBi6I12]2– cuboctahedra and Sn2+ or Bi3+ centered octahedra.

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α-Sn films grown on insulating (001) CdTe/GaAs

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α-Sn is an elemental topological material in which topological insulator - zero-gap semiconductor - Dirac semimetal transition can be realized by strain engineering [1]. Bulk α-Sn is stable only below 13.2°C. However, α-Sn phase can be stabilized above room temperature in a thin film form [2]. Recent experimental studies of this material have been mainly focused on α-Sn grown on narrow gap semiconducting substrates [3,4], which makes transport investigations problematic and limits potential application of this material [4].

In this work, 30-200 nm thick films of α-Sn are grown by the molecular beam epitaxy on (001) GaAs with CdTe buffer. Structural characterization performed by reflection high-energy electron diffraction (RHEED) (Fig.1(a)), atomic force and scanning electron microscopy as well as X-ray diffraction (XRD) proves high quality of obtained samples. XRD measurements reveale -0.1 % of in-plane compressive strains, the prerequisite for the Dirac semimetal (DSM) phase. α-Sn band structure is studied by angle resolved photoemission spectroscopy (ARPES) (Fig.1(b)) as a function of both temperature and film thickness. It is shown by ARPES that the prepared samples possess DSM phase in the thickness range 30-200 nm and in the temperature range 10-300 K. The presence of the DSM phase is further confirmed by magnetoresistance measurements. Negative longitudinal magnetoresistance (NLMR) is observed in a wide temperature range (1.6-90 K). Pronounced Shubnikov–de Haas oscillations confirm structural perfection of grown layers (Fig.1(c)).

Our results provide an important platform for further reliable investigation of transport properties and possible application of α-Sn in spintronic devices [4].

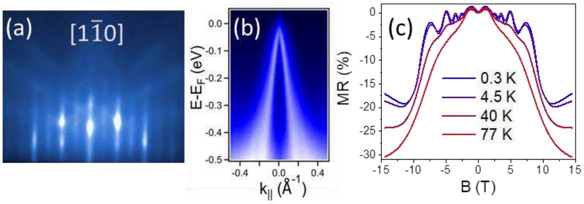

Fig.1 (a) RHEED patern, (b)ARPES spectrum and (c) NLMR of α-Sn film.

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Down-conversion luminescence of $Bi_2ZnOB_2O_6$ single crystals doped with Yb^{3+} and Er^{3+} ions

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$Bi_2ZnOB_2O_6$ single crystals doped with selected RE^{3+} ions are characterized by high values of nonlinear optical coefficients as well as the effective luminescence of excited RE^{3+} ions, which make this system a unique candidate for NIR to VIS laser converters. Such bi-functional materials, in which the laser effect and the non-linear optical phenomena occur simultaneously inside the same host are very attractive for the new generation laser devices. The crystals were shown to have high SHG and THG efficiency, comparable with those of well-known crystals such as BBO, KDP, KTP, which makes them very attractive materials for NLO applications [1,2]. The investigated $Bi_2ZnOB_2O_6$ nonlinear optical single crystals doped with Er^{3+} and Yb^{3+} ions were grown by the Kyropoulos method from stoichiometric melt. The Raman investigation showed the low phonon energy of $Bi_2ZnOB_2O_6$ host matrix associated to the vibrations of BO_3, BO_4, ZnO_4 and BiO_6 molecular groups, which allow effective phonon assisted energy transfer between Yb^{3+} and Er^{3+} ions [3]. The 1532 nm emission of $Bi_2ZnOB_2O_6$:Yb^{3+}/Er^{3+} single crystals, associated with the $^4I_{13/2} \rightarrow {}^4I_{15/2}$ transition of Er^{3+} ions, was excited at 380 nm (by Bi^{3+} ions), 488 nm (by Er^{3+} ions) and 980 nm (by Yb^{3+} ions) and efficient Yb^{3+} sensitization of Er^{3+} emission was observed [4]. The effective luminescence of exciting Er^{3+} ions in $Bi_2ZnOB_2O_6$ single crystals as well as excellent nonlinear optical properties of the $Bi_2ZnOB_2O_6$ host suggest that the investigated system can be very useful for new integrated optical converters.

Acknowledgements: This work was supported by the Research Project of the Polish Ministry of Sciences and Higher Education: 0511/SBAD/2251.

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Optical properties of Bi_3TeBO_9 ceramics doped with Yb^{3+}/Er^{3+} ions

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The nonlinear optical Bi_3TeBO_9 single crystal shows high effectiveness of the second (SHG) (20 times higher than KDP materials) and third (THG) harmonic generation [1]. Moreover, after doping with rare earth ions (RE^{3+}) Bi_3TeBO_9 matrix exhibit efficient luminescence [2]. The investigated $Bi_3TeBO_9:Yb^{3+}/Er^{3+}$ powders were obtained by means of the the modified Pechini method. The XRD measurements confirmed their hexagonal structure of $P6_3$ space group [1-3]. The samples of $Bi_3TeBO_9:Yb^{3+}/Er^{3+}$ ceramics were prepared under various preassure: 2, 4, 6 and 8 GPa. In this work the vibrational properties of $Bi_3TeBO_9:Yb^{3+}/Er^{3+}$ ceramics were studied by Raman spectroscopy. The up-conversion luminescence of $Bi_3TeBO_9:Yb^{3+}/Er^{3+}$ ceramics were measured in VIS spectral range under the excitation at 980 nm (Fig.1). The results show that investigated RE^{3+} doped ceramics may be potentially used in miniaturize optoelectronic devices.

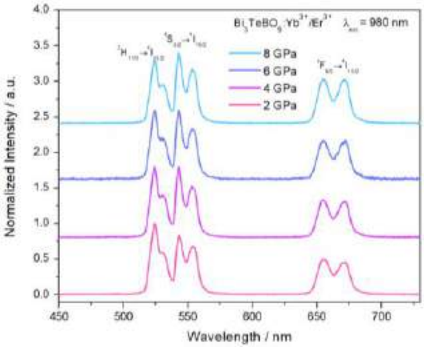

Fig.1 Emission spectra of Bi3TeBO9:Yb3+/Er3+ ceramics with different pressure under 980 nm excitation, recorded at 300 K

Acknowledgement: This work was supported by the Research Project of the Polish Ministry of Sciences and Higher Education: 0511/SBAD/2251.

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Topological insulators and eutectics at a crossroads

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Three-dimensional topological insulators attract great deal of interest due to their potential use of the topologically protected gapless surface states in topological spintronics and quantum computation [1]. However, challenges such as the high sensitivity of the surface states to the atmosphere, the low surface-to-volume ratio, and the need for various material heterojunctions currently limit the application of these materials [2]. Here, we report successful fabrication of the topological insulator heterostructures by an easy, fast and single-step process, which could meet all those challenges and pave the way for exploring other exotic phenomena in the near future. Utilizing directional solidification different topological insulator based eutectic composites were produced, where two crystalline phases are combined in a structured form with joined interfaces. The material exhibits lamellar micro/nanostructures with atomically smooth interfaces. Existence of the metallic surface states and the formation of p-n junction have been confirmed throughout specific characterization methods.

The authors thank ENSEMBLE3 Project (MAB/2020/14) which is carried out within the International Research Agendas Programme (IRAP) of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund and Teaming Horizon 2020 programme (GA. No. 857543) of the European Commission; the TEAM/2016-3/29 Grant within the TEAM program of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund.

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C-9 *Tuesday 21.06.2022, 15:00-15:15*

Crystal Growth and Unconventional Magnetism in $Pr_3Fe_3Sb_7$

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Rare earth and transition metal antimonides have widely been studied for their rich phase diagrams and diverse magnetic properties due to the interplay of 4*f* and 3*d* electrons.[1-3] Nasir *et al.* firstly mentioned unusual magnetization in the intermetallic $Nd_3Fe_3Sb_7$ but did not investigate it systematically.[4] We report on the synthesis and crystal growth of large, needle-like crystals of isostructural $Pr_3Fe_3Sb_7$ via flux growth technique, which shows equally complex magnetic properties.

Fe and Pr arrange in pseudo-one-dimensional substructures in close proximity. At room temperature, the Fe long-range order dominates the compounds behavior. However, below 50 K, the exchange interaction between the substructres initiates a strong temperature dependence of the magnetization showing compensation and even reversal of the overall magnetic moments direction. Powder neutron diffraction and magnetization measurements on single crystals reveal the complex Fe-Pr interaction, which is characterized by an antiparallel ordering and strong mangnetocrystalline anisotropy at low temperatures.

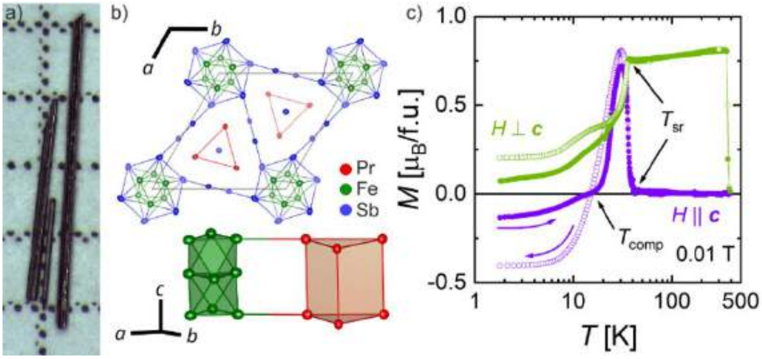

Fig.1 Single crystals of Pr3Fe3Sb7 (a). The crystal structure projected along the c-axis with details of the Fe and Pr substructure (b). The magnetization data measured on a single crystal displays magnetic compensation and negative magnetization (c).

We acknowledge financial support by the DFG and the Würzburg-Dresden Cluster of Excellence ct.qmat.

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Enhanced optical effects in doped plasmonic materials fabricated by crystal growth techniques

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Here, we demonstrate optically active volumetric materials obtained with micro-pulling down method. By applying NanoParticle Direct Doping Method, nanocomposites with plasmonic properties are fabricated, which allows us to observe enhanced optical features.

New generation of plasmonic materials are manufactured by NanoParticle-Direct Doping method developed in our laboratory. Possibility of direct introduction of plasmonic particles lets us easily dope glasses with NPs of various electromagnetic properties, thus tuning LSPR to enhance the targeted effects, e.g. PL of quantum dots. The scope of interest also covers eutectic crystals with plasmonic dopants that demonstrate unusual optical effects.

Combining research on both fabrication and characterization of the novel materials with unusual electromagnetic properties may result in development of low-cost photonic devices with enhanced functionalities.

Acknowledgements: The authors thank the TEAM Project (TEAM/2016-3/29) and International Research Agenda Programme (MAB/2020/14) of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund.

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Introduction to the Centre of Excellence ENSEMBLE^3 Sp. z o.o. TO BUILD THE BASIS FOR FUTURE PHOTONICS

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ENSEMBLE^3 Centre of Excellence, located in Warsaw, Poland builds on the pioneering work of Prof. Czochralski and following world-leading expertise. Concept of the Centre has been created jointly by the following renowned institutions from Poland, Germany, Italy, and Spain: the Łukasiewicz Research Network Institute of Electronic Materials Technology and the University of Warsaw (Poland), the Karlsruhe Institute of Technology (Germany), the Sapienza University of Rome (Italy), and the Nanoscience Research Centre nanoGUNE(Spain).

Our Centre is a place fostering innovation and international collaboration by providing infrastructure and know-how for both young and advanced researchers with pioneering ideas.

ENSEMBLE3 gathers the expertise, know-how, and facilities in the field of crystal growth of single crystals of oxides, fluorides, III-V semiconducting compounds, SiC, and organic materials. The available growth methods include Czochralski, Liquid Encapsulated Czochralski, floating zone, micro-pulling down and others.

Based on unique expertise, materials, and apparatus we offer: joint research and development in the field of novel materials for photonics; crystalline materials technology development; on-demand designed materials including crystal boules, wafers, fibres, and elements; material characterization.

Acknowledgement

We thank the ENSEMBLE^3 Project (MAB/2020/14) which is carried out within the International Research Agendas Programme (IRAP) of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund and the Teaming Horizon 2020 programme (GA. No. 857543) of the European Commission for supporting the ENSEMBLE^3 Centre.

Polarization selection properties of donor-doped ZnO multilayers

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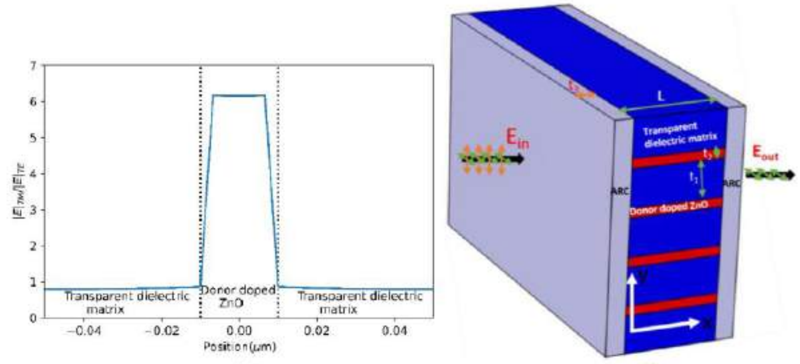
Recently, transparent conducting oxides, such as donor-doped ZnO, indium tin oxide etc., due to extreme electric field enhancement near the epsilon near zero (ENZ) wavelength, have been used in high harmonic generation [1], ultrafast switching [2], modulation [3], etc. In this paper, we show a strong electric field enhancement for the transverse magnetic (TM) polarized incident beam compared to the transverse electric (TE), in the donor doped ZnO layer near its ENZ wavelength. Harnessing this feature, we propose the design of a polarizer based on donor doped ZnO multilayer in a transparent dielectric matrix. We observed oscillations in the transmittance due to high reflection at the facets of the structure. In order to reduce the oscillations, we considered an antireflection coating (ARC) of glass at both facets of the structure. The polarizer performance is calculated using FEM simulations and we found transmittance >80% under TE polarized light, and a TE/TM polarization extinction ratio of more than 1000 in the telecommunication wavelength range 1230- 1460 nm, for appropriately chosen structural parameters.



(a) (b)

Fig.1 (a) Enhancement of electric field for TM polarization compared to the TE polarization, in the donor doped ZnO layer and (b) Schematic of the proposed design.

The authors thank the ENSEMBLE3 Project (MAB/2020/14) which is carried out within the International Research Agendas Programme (IRAP) of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund and the Teaming Horizon 2020 programme (GA. No. 857543) of the European Commission.

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Superior electrochemical energy storage and conversion properties of Bi_2CuO_4-Bi_2O_3 eutectic

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Abstract: Bi_2CuO_4-Bi_2O_3 eutectic (BCBE) composite was prepared by the micro pulling down method. The eutectic rod was cut and polished. Samples with different thickness were prepared and their potential for electrochemical applications such as supercapacitor and catalyst was investigated. We found three times increase in the current response when the sample thickness was reduced from 600 to 200 μm. BCBE exhibited very high areal capacitance of ~78 mF/cm^2 at 10 mV/s scan rate. BCBE showed redox nature in 6 M KOH electrolyte. Inspite of the faradic nature, the cylic voltammetry (CV) remained undistorted at very high scan rate of 500 mV/s (Fig. 1). At the same time, we also used BCBE as the catalyst for electrochemical hydrogen evaluation reaction (HER). BCBC demonstrated very low overpotential and high current response at a low onset potential. The superior supercapacitor and HER properties suggested that BCBE is suitable for next generation energy storage as well as energy conversion applications.

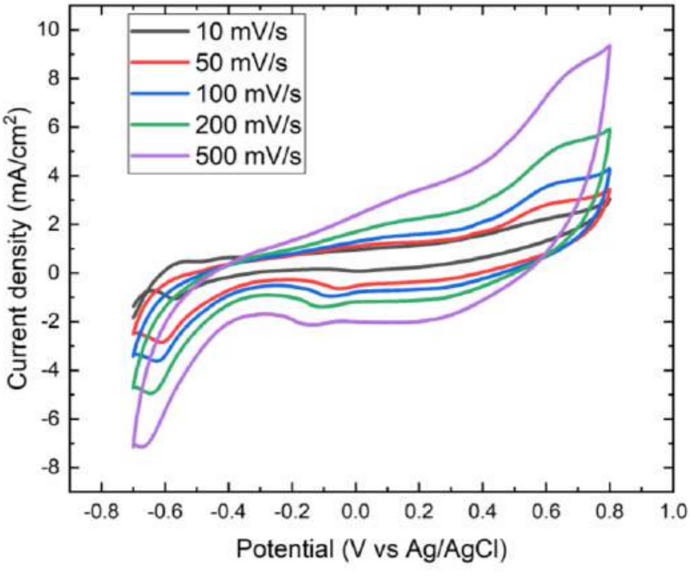

Fig.1 Three-electrode cylic voltammetry plots of BCBE at different scan rates.

Acknowledgements: The authors thank the ENSEMBLE3 Project (MAB/2020/14) which is carried out within the International Research Agendas Programme (IRAP) of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund and the Teaming Horizon 2020 programme (GA. No. 857543) of the European Commission.

Influence of crystal growth conditions on the superconductivity in Ce_nPdIn_{3n+2} (n = 2, 3) phases

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Cerium-based intermetallics belong to the most investigated compounds in solid state physics. It is mainly due to intriguing electronic properties they exhibit. Among a large variety of phenomena observed in those compounds, one may enlist complex magnetic ordering, non-Fermi liquid features, heavy-fermion behavior, spin and valence fluctuations, superconductivity, etc. Performed in recent years extensive studies of ternary cerium indides, especially a family with the general formula $Ce_mT_nIn_{3m+2n}$, showed that superconductivity is a commonly observed phenomenon in this group of materials. While many experimental data on heavy-fermion superconductivity have been collected on cobalt, rhodium and iridium-based compounds, their palladium and platinum-bearing counterparts have only been roughly examined due to lack of high-quality samples.

Up to now, the only applied method of obtaining Ce_nPdIn_{3n+2} (n = 2, 3) single crystals is the growth from indium flux. This technique usually leads to forming crystals of small dimensions, not exceeding 1 mm^3. Moreover, it often yields crystals with macroscopic inhomogeneities [1]. This drawback may be caused by several factors: i) from one initial stoichiometry it is possible to grow several different phases ($CeIn_3$, Ce_2PdIn_8, Ce_3PdIn_{11}) depending on the temperature range used during the synthesis; ii) the growth of the ternary phases takes place only in a very limited temperature interval (different for each compound); iii) due to the similar crystal structure of all the $Ce_mT_nIn_{3m+2n}$ compounds and almost perfect match of the lattice parameter a (= 4.6894 Å [2], 4.6931 Å [3] and 4.6846 Å [4] for $CeIn_3$, Ce_2PdIn_8 and Ce_3PdIn_{11}, respectively), previously grown crystals of one compound may constitute a seed and substrate for the growth of another of these phases.

In our ongoing crystal growth studies of Ce_nPdIn_{3n+2} compounds, we had addressed these problems and by varying growth recipes, we were able to selectively obtain large single crystals of Ce_2PdIn_8 and Ce_3PdIn_{11} phases. Interestingly, the conditions applied during the syntheses significantly affect the superconducting properties of these materials.

This work was financially supported by the National Centre of Science (NCN, Poland) within a research grant MINIATURA 5 no. 2021/05/X/ST5/00592

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Synthesis and characterization of selected MTPn compounds

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The discovery of topological materials has opened up a new frontier in the study of condensed-matter physics. Theoretical predictions have brought on renewed interest in materials that, in many cases, have been known and thought to be fully characterized for years. Recently, various topological phases have been predicted in the members of MTPn family, where M – Ca, Sr, Ba, T – Cu, Ag, Au and Pn – As, Sb, Bi. However, the experimental confirmations are hindered by the lack of high quality single-crystal samples, which are necessary for detailed characterization.

An improved synthesis protocol for several Ag-based members of the MTPn family will be presented here, along with the description of crystal structure and composition, as well as the results of heat capacity and electronic transport measurements.

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Magnetic phase diagrams of UPd_2Si_2

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Ternary uranium silicides with overall composition UT_2Si_2, where T is a *d*-electron transition metal, crystallize with tetragonal unit cells of the $ThCr_2Si_2$ type (s.g. *I*4/*mmm*) or the closely related $CaBe_2Ge_2$ type (s.g. *P*4/*nmm*). Competition between crystallization of the two polymorphs may result in a structural instability that strongly influences the bulk physical characteristics [1]. UPd_2Si_2, adapting the $ThCr_2Si_2$ type structure, exhibits complex magnetic phase diagram constructed for magnetic field applied along the tetragonal c axis. It comprises three ordered phases, namely incommensurate longitudinal spin wave (ICLSW), ferrimagnetic (FiM) and simple antiferromagnetic (AFM) [2,3]. Remarkably, in high magnetic fields, paramagnetic (P), FiM and ICLSW phases, meet each other at a point [2,3] that has been suggested to be a bicritical Lifshtz point (LP), whose "critical behavior is strikingly different from any other" [3,4].

The magnetic phase diagrams of UPd_2Si_2 reported in the literature, show some notable differences [2,3], presumably related to the structural instability of the compound, similar to those observed before in other UT_2Si_2 phases [1]. In order to clarify the discrepances, we synthesized several single crystals of UPd_2Si_2 using the Czochralski pulling technique in a tetra-arc furnace. Chemical composition and the crystal structure of each crystal were checked by means of energy-dispersive x-ray spectroscopy and x-ray diffraction perfomed on Laue backscattering and four-circle diffractometers. Their magnetic, electrical transport and thermal properties were characterized in wide ranges of temperature (2–300 K), and magnetic fields (up to 14 T).

We constructed the magnetic phase diagrams of the grown crystals and identified three main types of behavior, two of them being consistent with those reported in the literature [2,3]. In zero magnetic field, the crystals differ in terms of number of phase transitions and values of critical temperatures. However, n high magnetic fields, their properties are similar. In particular, for each crystal type, the P-FiM and FiM-ICLSW phase boundaries tend to merge as expected for the appearance of LP.

This work was supported by the National Science Centre of Poland grant no. 2018/31/D/ST3/03295.

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Morphology of Cd and Te inclusions and their impact on the stresses and internal electric field distributions in (Cd,Mn)Te crystals

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(Cd,Mn)Te crystals are currently being studied for applications in X-ray and gamma radiation detectors. This application requires high volume crystals, e.g., 10×10×3 mm3 or more, with the best crystal quality. Any crystal structure defect, such as grain boundary or inclusion, influences the charge carrier transport. The presence of inclusions is typical in materials grown by the Bridgman method. The aim of this study was to analyze the influence of cadmium and tellurium inclusions on the stresses and internal electric field distributions in (Cd,Mn)Te crystals. For this purpose, two types of (Cd,Mn)Te crystals were used: (1) a crystal grown under Cd-excess and (2) under Te-excess, so that Cd or Te inclusions can be examined, respectively. Infrared and electron microscopic observations reveal a different morphology of the Cd and Te inclusions. The Te inclusion is spherical. Sometimes, however, a different morphology is observed, depending on the orientation of the sample. Meanwhile, the Cd inclusion located in the (111) plane produces a star-like defect, which consists of a round core and six branches that radiate from the core. Electron Backscatter Diffraction measurements show that both Cd and Te inclusions cause a stress field in their vicinity [1]. Due to the presence of microcracks, the value of relative stresses is lower in the vicinity of Cd inclusion than in the case of Te. The mobility-lifetime products of the (Cd,Mn)Te crystals are measured by the non-contact method, using the time dependend charge principle. Their values indicate inferior charge transport properties in the crystal with Cd inclusions. Next, by means of the Pockels effect imaging, the internal electric field was analyzed. Only grouped Te inclusions affect the electric field in the (Cd,Mn)Te crystals [2].

The authors would like to gratefully acknowledge Marcin Dopierała, Janusz Gdański, Stanisław Jabłoński, Michał Kochański, Adam Marciniak and Marek Zubrzycki for their technical support during experiments.This work was supported by the Polish National Centre for Research and Development through grant No. TECHMATSTRATEG1/346720/8/NCBR/2017.

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Investigation of pulsed-laser deposition of $LuFeO_3$ by in-situ synchrotron x-ray diffraction

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We investigated the PLD of epitaxial layers of hexagonal $LuFeO_3$ by measuring the X-ray diffraction intensity in the quasiforbidden reflection 0003 *in situ* during deposition. The time dependence of the diffracted intensity exhibited characteristic oscillations, from which we determined the growth rate and the time evolution of surface roughness. The roughness is described by the scaling exponent β occurring in standard models of growth based on stochastic growth equations and a random fractal approach. Subsequently we modelled the growth using a kinetic Monte Carlo model. While the experimentally obtained scaling exponent decreases with the laser frequency, the simulations provided the opposite behaviour. We demonstrate that the increase of the surface temperature caused by impinging ablated particles satisfactorily explains the recorded decrease in the scaling exponent with the laser frequency.

We compared the results of the kinetic Monte-Carlo simulations with simulations carried out using a phenomenological rate-equation model and we showed that the phenomenological model correctly describes the growth kinetics.

The work was supported by the Czech Science Foundation (Project No. 19-10799J) and by the project NanoCent financed by European Regional Development Fund (ERDF, Project No. CZ.02.1.01/0.0/0.0/15.003/0000485). The additional funding by the German Research Foundation within the framework of the Projects SCHN 669/1-1 and BA 1642/8-1 is gratefully acknowledged.

C-19 *Thursday 23.06.2022, 16:25-16:40*

Cost-efficient methods to grow high-melting-point oxide crystals from melt

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High-melting-temperature oxide crystals are demanded for laser, scintillator, and other optoelectronic applications. Such bulk crystals are grown from the melt at high temperatures up to ~2500 °C in an inert gas atmosphere, which require the involvement of precious metal (Ir, Re) crucibles and parts in the process. Following various estimations, the cost of Ir crucibles comprises up to 50% of the total cost of crystals, and this rate sharply increases in recent decade owing to the high demand for Ir on the market. The processes involving cheaper crucible materials, or crucible-free methods have been developed by different teams [1-5].

In this report, we overview our recent achievemens in growth of sesquioxide, rare earth aluminate and silicate single crystals in Ar+CO atmosphere using Mo and W crucibles, which are ~1000 times cheaper compared to precious metals. Bulk $Y_3Al_5O_{12}$- and $Lu_3Al_5O_{12}$-based garnet and $(La,Gd)_2Si_2O_7$:Ce pyrosilicate crystals were successfully obtained by the Czochralski method, while Y_2O_3 and $(Y,Sc)_2O_3$ sesquioxides were grown by the VGF. We have also crystallized Y_2SiO_5:Ce crystals by the Bridgman method. Tests of optical and scintillation parameters confirmed that the obtained scintillators (except Y_2SiO_5:Ce) by their performance are not behind the analogs grown by the conventional technology in Ir crucibles.

Further development of single crystal production technologies and reduction of their cost requires scaling up of crystals, which would allow producing large scintillation detectors for the absorption of high-energy particles, or a large number of small pixelated crystalline elements in one technological cycle. This aspect is addressed on the example of Czochralski growth of large $Y_3Al_5O_{12}$:Ce crystals with a weight of up to 2 kg in W crucibles.

This work was supported Narional Academy of Science of Ukraine Project “Carbon-2”, International Research Project “ScintLab” of CNRS, France, and French-Ukrainian bilateral project “Dnipro”(agreement with Minitstry of Science and Education of Ukriane M/36-2021 by 16. 11.2021), “ENSEMBLE3 project (GA no. MAB/2020/14) carried out within the International Research Agendas program of the Foundation for Polish Science and Teaming for Excellence project (GA no. 857543)".

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C-20 *Thursday 23.06.2022, 16:40-16:55*

Highly efficient alcohol detection by SPR based sensors

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Amongst all kinds of optics, and optoelectronics approaches incorporated in the sensing area, the usage of surface plasmon resonance (SPR) seems to be one of the most promising techniques of detection [1]. Optimized thermal annealing of thin metal films can lead to optically active, isolated nanoislands formation in a cost-effective way. Such an easily controllable process can lead to robust plasmonic platforms with the desired properties formation [2]. These plasmonic properties of nanostructures depend on dielectric properties of the medium, that the structure is put in, which makes them uniquely attractive in gas or liquid detection. This approach is definitely simpler and seems to own a better chance of being implemented in applications area than broadly found in literature refractive index based sensing [3].

Studied plasmonic nanostructures were prepared through thermal dewetting of thin Au film sputtered on a glass substrate. Such prepared plasmonic platforms were examined for their usability as alcohol sensors. A sensitivity assessment test performed on the basis of measurements in various concentrations of ethanol showed linear dependence of plasmonic band position in correlation with ethanol concentration.

Our studies show that such simply, cost-effective synthesis technique can lead to high quality sensing devices obtainment, which might be attractive for commercial applications.

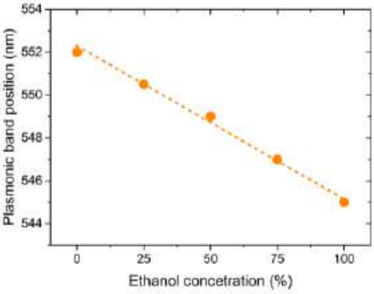

Fig.1 The dependence of plasmonic band position in correlation with alcohol concentration.

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Effects of boron doping on the electrical, optical and morphological properties of nanocrystalline diamond sheets: Tuning the diamond-on-graphene vertical structure

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Diamond sheets are of considerable interest as potential transparent and flexible electronic devices [1,2]. However, there is a significant lack of knowledge regarding the effects of boron incorporation on the electrical, morphological and optical properties of freestanding boron-doped diamond sheets.

In this work, we analyze the properties of nanocrystalline diamond microsheets as a function of boron doping. Freestanding microsheets with a thickness of 1.3 ± 0.3 µm were obtained by spontaneous delamination following growth on tantalum substrate in a microwave plasma-enhanced chemical vapor deposition reactor. Each sample was grown with a different [B]/[C] ratio (up to 20 000 ppm) in the gas phase.

The lower doped samples show p-type semiconductor character (nearest-neighbor hopping and variable-range hopping are observed), while the highest-doped sheet with [B]/[C] = 20 000 ppm exhibits the metallic conductivity. With increasing boron concentration, a strong reduction in grain size and a decrease in the diamond phase are observed. Moreover, boron incorporation into the diamond microsheets shifts the position of the sp^3 peak towards lower frequencies.

As a proof of concept, we present a diamond-graphene junction. The heterojunction with the low boron concentration sheet resembles a Schottky junction behavior, while an almost Ohmic contact response is recorded with the highly doped BDD sheet

Our results can be a stepping stone in the production of diamond-based flexible electronic devices.

M.R. acknowledges the financial support of the National Agency for Academic Exchange under the Iwanowska Programme (PPN/IWA/2019/1/00091/U/00001). D.H.S acknowledges funding by the KIND postdoctoral fellow program of the Kavli Institute of Nanoscience Delft. J.G.B acknowledges the Dutch Research Council (NWO) for funding through the Open Technology Programme (project no. 16361). The financial support from the Gdańsk University of Technology under the Plutonium grant (DEC-2/2020/IDUB/III.4.3/PU) is also acknowledged.

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C-22 *Friday 24.06.2022, 11:50-12:05*

Influence of native substrate misorientation on structural properties of InGaN on GaN pseudo-substrate

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The idea of using InGaN templates for the epitaxial growth of InGaN-based devices has emerged last years. InGaN pseudo-substrates with lattice parameters bigger than conventional GaN substrate could be obtained by enabling the strain relaxation of InGaN epitaxial layers deposited on GaN substrates. The plastic strain relaxation of InGaN layers grown on (0001)-oriented GaN is carried out by nucleation of (**a+c**)-type dislocations gliding on $\{1122\}$ pyramidal planes and forming trigonal network of misfit dislocations along $\langle\bar{1}100\rangle$ directions at the InGaN/GaN interface [1]. The particular $\langle\bar{1}100\rangle$ direction is the common intersection of the interface with two mirror $\{1122\}$ glide planes. Then the (**a+c**)-type misfit dislocations lying along this direction may have one of two Burgers vectors, varying in the sign of the **c**-component. However, it has been evidenced that the majority of dislocations lying along the particular $\langle\bar{1}100\rangle$ direction have the same Burgers vector indicating preferential dislocation formation mechanism [2].

In this work, we study the influence of substrate misorientation on preferential dislocation formation and how it affects structural properties of relaxed InGaN layers. 50 nm and 100 nm thick $In_{0.19}Ga_{0.81}N$ layers were grown by nitrogen plasma assisted molecular beam epitaxy on bulk (0001) GaN substrates with various miscut angles (0.3°, 0.8° and 1.3° toward $\langle\bar{1}100\rangle$ or $\langle 1120\rangle$ direction). Structural analysis was done using high-resolution X-ray diffractometry, cathodoluminescence imaging and transmission electron microscopy.

We demonstrate that InGaN layers grown on misoriented substrates relax by preferential formation of (**a+c**)-type misfit dislocations. The substrate misorientation changes the resolved shear stresses in each slip system, resulting in different nucleation ratio in each dislocation set. We observe preferential dislocation formation that could be separated into two kinds. The preferential glide on one $\{1122\}$ plane from mirror related pair leads to the layer tilt with respect to the substrate. An additional tilt of the InGaN layer with respect to the GaN substrate reduces the final misorientation of the InGaN pseudo-substrate. In turn, the preferential formation of dislocations in particular $\langle\bar{1}100\rangle$ sets results in irregularity of misfit dislocation network. It leads to the in-plane anisotropy of the layer. To preserve a wurtzite symmetry of the InGaN pseudo-substrate, low misorientation of the initial GaN substrate is required.

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Influence of diffusion of point defects on decomposition of the InGaN/GaN QWs.

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In our study, we focus on the role of the point defects diffusion from the layers below the InGaN QWs, on their optical and structural properties but most of all on their thermal stability. The motivation for examining point defect diffusion was that the thermal decomposition of indium-rich (around 20%) quantum wells grown by MOVPE method always starts from the first grown QW [2].

In order to investigate this topic two samples were prepared - one Si doped GaN layer grown on standard sapphire template and second one, analogous, but Mg doped. These two samples were divided into two parts and then one part was implanted with He ions. Energies and doses were chosen to introduce only point defects into doped GaN layers. STEM studies confirm that the used He ion atom implantation fluxes, does not cause GaN amorphization or the formation of extended and planar defects. Changes in the structure and also in recombination mechanism after implantation were confirmed by High Resolution X-Ray Diffraction (HRXRD) and Photoluminescence (PL) spectra. To better understand the nature of the resulting defects, the implanted samples were examined by Positron Annihilation Spectroscopy (PAS). The S parameter values of He implanted GaN layers show that the ion bombarding produces Ga vacancies and their complexes at density of 10^{19} cm^{-3} or more (saturation of positrons).

On such prepared Si and Mg doped GaN layers implanted with He ions and unimplanted, $In_{0.2}Ga_{0.8}N$/GaN QWs were grown in one epitaxial process. To investigate the impact of point defects diffusion, on structural and optical properties as well as thermal decomposition of this InGaN/GaN QWs, the grown structures have been subjected to a series of annealing at temperatures 900˚C, 920˚C and 940˚C. HRXRD 2theta/om scans, STEM images and PL spectras obtained after annealing indicate that the QWs grown on the implanted layers, i.e. with high V_{Ga} density degrade more rapidly at a lower annealing temperature compare to QWs grown on unimplanted layers. At elevated temperatures, we also observe faster deterioration of the optical properties of the QWs grown on implanted GaN:Si layer [3].

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Formation mechanism and characterisation of alloyed plasmonic nanostructures

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Metallic nanoparticles have been attracting the attention of scientists for over a decade. It is caused by their unique catalytic and optical properties. In particular, collective oscillations of conductive electrons, known as plasmon resonance, enable many applications in various fields, such as optoelectroics, photocatalysis, photovoltaic devices, surface-enhanced Raman scattering and even anti-cancer therapy [1, 2]. This group includes alloyed nanostructures, which are currently very popular. They are nanomaterials composed of two, or more, various metal elements. Their uniqueness is evidenced by the attributes that are typically a combination of properties derived from metal amalgams. These properties, and thus applicability of such nanoparticles, are related not only to their size and shape, as in the case of monometallic nanoparticles, but also to their chemical composition and structure [3]. Hence, proper control over the fabrication of such systems poses a significant experimental challenge.

Here, we present the results of the investigation of initial fabrication parameters and experimental conditions influence on the formation and optical properties of AuAg nanostructures. Nanoalloyed, hemispherical nanostructures, with dimensions in a range of 20 nm- 60 nm were formed as a result of dewetting of Au/Ag thin layers. We used a thermal treatment with temperatures well below theirs melting temperature for fabrication [4]. Structures were deposited on Corning 1737 glass and silicon substrates. For the surface morphology studies, SEM and TEM measurements were performed. The structure of plasmonic nanostructures was investigated using XRD, as well as XPS methods, while plasmon resonance was observed by UV-VIS spectroscopy.

Our investigations confirmed formation of AuAg nanoalloys. Optical measurements of manufactured nanostructures showed a tunable optical properties depending on its composition.

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AlGaN composition determination in GaN based structures grown on silicon using HRXRD.

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A simple method for the determination of the AlGaN composition in GaN based structures grown on silicon is shortly shown and discussed in some details. The stability and the simplicity of the method, based on the properties of the (205) AlGaN reflection, are reviewed and applied to a case study. In fact it can be shown that the d-spacing of this particular reflection of the AlGaN alloy is quite insensitive to the strain status of the layer, this allows to extract quite directly the AlGaN composition without a full strain analysis of the layers. In particular wafer mapping of the AlGaN composition are greatly simplified with this approach. Different measurement strategies are shown and discussed especially taking advantage of the progress in detector technology.

Posters

Poster PS-1

Tuning the broadband optical properties of large-area nano- and meta- materials

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Materials displaying tailored broadband optical properties are focusing the interest of researchers and technologists, for the design of more robust and efficient devices for applications in light harvesting, multispectral camouflage, energy management, cloaking, or optical elements [1-3]. Considering recent reports, properties such as tailored broadband absorption, reflection, or polarization can be achieved by tuning some parameters e.g. structure and composition of nano- and meta- materials and post-growth treatment [4,5]. Moreover, remarkable performances in broadening spectrum, enhanced resonance response and SERS (1 surface-enhanced Raman scattering are acceded by disorder and multiphase materials [6-9]. To make a step toward practical, real-world applications, it is needed to have such materials fabricated with a large-area using [4,10]. Furthermore, obviating such expectations with complex internal structures is a complicated issue through top-down methods such as laser lithography. Nevertheless, eutectic solidification and self-assembly manners are promising techniques to fabricate materials with intricate internal structures [10].

Here, we report on our project which involves the characterization of the optical response of large-area nano- and meta- materials promising for broadband optical applications. A special emphasis is made on oxides, metals, and composites. These materials are characterized in a broad spectral range from the ultraviolet to the far infrared. Their broadband optical response and its tunability are discussed in relation with their structure and fabrication and processing conditions.

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Poster PS-2]

Tin-doped thin diamond film synthesis using microwave plasma chemical vapour deposition

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This research focuses on the study of the tin-vacancy (SnV) centers induced in a thin diamond film using microwave plasma chemical vapour deposition (MPCVD). Thin films were characterized with scanning electron microscope (SEM), Raman and photoluminescence spectroscopy.

Currently, SnV centers are fabricated mainly with Sn ion implantation and subsequently annealed [1] to incorporate Tin into the diamond lattice. Due to a sharp and strong zero-phonon line (ZPL) at 619 nm and long spin coherence times [2], Tn-vacancy centers in diamonds are a promising approach for quantum optics and quantum networking.

Diamond films with Tin-vacancies were created with CVD process using the following condition: a gas mixture of H_2, B_2H_6, and CH_4 with a total flow of 303 sccm, the pressure of 50 Torr, microwave power of 1300 W, microwave radiation 2.45GHz, the temperature of 700 °C and growth time of 4 hours.

Raman spectra showed highly-degenerated diamond with the addition of graphitic phases. Photoluminescence spectra exhibited a peak nearby 620 nm, which is considered SnV marker. Surface morphology in SEM images displays Tin spheres overgrown by diamond and carbon phases in size of a few micrometers as shown in Figure 1. Mechanism of tin incorporation in-situ during MPCVD growth, Tin donor role, and its concentration influence on diamond layer properties are cross-correlated and discussed.

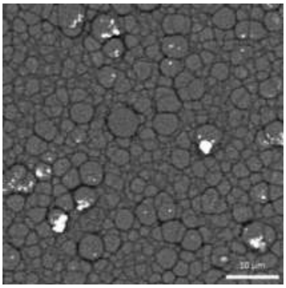

Figure 1. SEM image of produced MPCVD diamond thin film with tin addition to create tin-vacancy.

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Poster PS-3

The Curious Case of Black Titanium Oxide

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Titanium dioxide (TiO_2) has been enthusiastically studied as a light absorber, electron-transporting material and catalyst in different energy and environmental applications. The discovery of ''black'' TiO_2 (b-TiO_2) with visible and infrared absorption has triggered an explosion of interest due to the its great application potential for energy applications [1] [2]. After discovery of b-TiO2, its synthesis became a hot area in the current environmental perspective. Different synthesis strategies have been employed up to now [3], however, all these processes including hydrogenation, are multi-step and time consuming.

Here, b-TiO_2 crystal has been successfully grown from the melt, for the first time without a subsequent hydrogenation process. Electrical characterization of this material shows the resistivity as low as ~0.1 Ohm.cm. By selective annealing of the material, the electrical properties as well as the colour of the material, can be precisely controlled.

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Poster PS-4

Icosahedral phase synthesis in Al-Cu-Fe-REE system: rapid solidification and flux-grown monocrystals

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Quasicrystals are ordered structures that lack translational periodicity, which can lead to unusual and potentially promising physical properties. Although long-range spin coupling has rarely been observed in quasicrystals, recent findings of Tamura *et al.*[1] motivated us to search for new magnetic quasicrystals. We focused our search on interactions between the moments of the itinerant *3d* electrons of Fe and the localized *4f* electrons of selected rare-earth metals.

Phase equilibria in the aluminum-rich corner of Al-Cu-Fe-REE±B system were investigated to determine the icosahedral phase stability and the presence of accompanying magnetic phases. Pure elements were homogenized by arc-melting and the ingots were solidifed by cooling on a water-chilled copper block at rates on the order of $10\ K{\bullet}s^{-1}$. The microstructure, for example of a multi-phase Nd-bearing alloy that exhibited room temperature ferrimagnetism is shown in the Fig. 1. Subsequently, a flux-growth method was used to obtain mm-sized single-phase quasicrystal grains from base alloy melts with compositions $Al_{59-x}Cu_{37}Fe_4Yb_x$ (x=0.05, 0.50 and 1.00 at.%). The level of Yb doping in the icosahedral structure was found by EDS analysis to be 0.04±0.02 at.%,for any Yb content of the base alloy greater than zero. Excess Yb in the base alloy results in the formation of a secondary tetragonal phase, Al_8Cu_4Yb (*I4/mmm*), whose relative abundance and crystal size increase as Yb content increases. The latter phase has a stoichiometry close to Al_8Cu_5Yb (*Fm-3c*), which is composed of interconnected $[Al_8Cu_4]^{2-}$ icosahedra [2] and can be considered a quasicrystalline approximant.

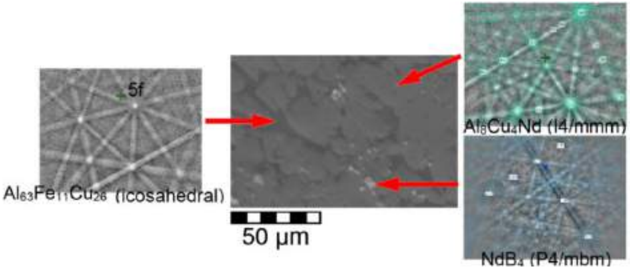

Fig.1 SEM micrograph of therepresentative Al-Cu-Fe-Nd-B alloy with corresponding EBSD patternsand phase composition from EDS

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Poster PS-5

Nanocomposite glasses co-doped with quantum dots, rare-earth ions and Ag nanostructures for a tuned light emission

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Materials that include several types of nanoemitters coupled with plasmonic metal nanostructures (NS) are gaining attention for their use in ultrafast optoelectronics, quantum information science and photovoltaics [1-3]. The combination of multiple types of nanoemitters (such as quantum dots - QDs - or rare-earth ions – RE) enables achieving tuned photoluminescence spectra. Thanks to their strong optical absorption and near-field enhancement properties, metal NS are useful to enhance the photoluminescence of nanoemitters, either by increasing the effective optical excitation cross-section, or by stimulating optical emission. Harnessing these properties to achieve a spectrally tuned and efficient photoluminescence from functional bulk glasses is needed for practical real-world applications. In this contribution, we present the ultraviolet-visible-near-infrared optical properties of light-emitting bulk nanocomposite sodium-borophosphate glasses doped with QDs of CdTe or CdSe/ZnS, RE ions of Pr^{3+}, and Ag NS that act as light emitters and plasmon sources, respectively. The glasses are prepared by the nanoparticle direct doping [4] method which utilizes the micro-pulling-down concept. The prepared samples are characterized by steady-state and time-resolved photoluminescence as well as by optical transmission measurements. We demonstrate tuned photoluminescence spectra thanks to co-doping of Pr^{3+} RE ions and silver NPs. Importantly, we show that Pr^{3+} ions induce a broadening of the visible emission to the near infrared region. The benefit of incorporating Ag NS is also discussed.

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Compendium of Natural Epsilon-Near Zero Materials and their Quality Factors

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Epsilon Near Zero (ENZ) materials is one of the most interesting group of metamaterials showing fascinating response to the electromagnetic waves and hence it creates a new realm for fabricating new optical and optoelectronics devices [1]. Such behaviors basically stem from interaction of light with possible resonances in a substance altering the dielectric permittivity [2]. Therefore, knowing a wide range of materials with such a capability is necessary and it enables us to design devices with desired operational wavelengths and performance. In this work, a complete set of natural materials, including metals, semiconductors, oxides, halides and other materials, which have dielectric permittivity around zero, together with different quality factors will be presented. We will discuss different quality factors for various applications and eventually introduce best candidates for those applications. Ultimately, this study provides a tool the metamaterials and materials science community to design ENZ-based devices with high efficiency and desired characteristics.

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Poster PS-7

Combining Bi and Ag in Bi_2O_3:Ag metamaterials for switchable plasmonics and Raman signal enhancement

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Bi_2O_3:Ag nanostructured metamaterials grown by the directional eutectic solidification method show a great potential to achieve plasmonic properties in a volumetric material that can be produced on a large scale [1]. In nitrogen annealed materials, plasmonic properties are dominated by resonances in the Ag nanoparticles, which enhance the Raman signal of the matrix and the photoluminescence properties of rare-earth ions when added to the matrix [2]. The plasmonic properties of these materials can be spectrally tuned by suitable annealing treatments in air or hydrogen. Such treatments are prone to altering the composition of the matrix, which could be partially reduced to induce the formation of Bi nanostructures in a Bi_2O_3 environment, or Bi nanolayers at the surface of the Ag nanoparticles to form Bi@Ag core-shell nanostructures [1]. Bi is an “alternative” plasmonic material, which has the capability to support plasmon-like resonances in the ultraviolet-visible, which can also result in Raman signal enhancements. Furthermore, it is a phase-change material, the plasmonic properties of which can be switched upon varying temperature. Here, we explore the potential of combining Ag and Bi nanostructures in a single metamaterial to enhance its properties. In particular, we discuss the effect and possible advantages of dispersing Bi and Ag nanostructures in a Bi_2O_3 matrix, and the effect of Bi@Ag core-shell nanostructure formation, on the optical, thermo-optical and Raman properties of the metamaterial. These results pave the way to the design of hybrid systems harnessing both traditional and unconventional plasmonic nanostructures.

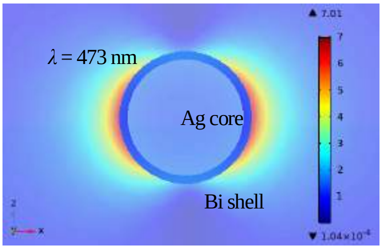

Fig.1 Electric field distribution of single Ag core (40 nm) and Bi shell (thickness 5 nm) nanostructure in air medium.

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Poster PS-8

Optical resonances in quantum nanostructures

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Nanostructures displaying plasmonic or high refractive index properties are appealing because of their capability to confine or guide light at the nanoscale, which is of interest for applications as diverse as solar energy conversion, non-linear optics, or nanophotonic circuitry, among others. However, the performance of standard nanostructures for plasmonics and high refractive index photonics is far from optimal. For instance, standard plasmonic nanostructures consisting of Ag or Au suffer from significant optical losses; standard high refractive index nanostructures consisting of Si, Ge or GaAs display refractive index values around only 4 that limit their potential. Novel nanostructures harnessing paradigms of quantum physics and compositional control are being considered to achieve unprecedented plasmonic properties and much higher refractive index values (near 10). [1,2] Among this new class of nanostructures, those consisting of Bi and its compounds are particularly appealing because of their capability to support a broad variety of optical resonances displaying either metal-like or dielectric-like features with outstanding spectral and spatial properties. Here, to assess the potential of these novel nanostructures, we analyze the spatial and spectral properties of their optical resonances for different compositions and geometries, either when nanostructures are free-standing or are integrated in multilayer systems. We study the effect of these parameters on the light-nanostructure coupling efficiency and optical spectra, to find the best conditions for optimal properties.

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Poster PS-9

Superconductivity in osmium-based Laves phases

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Laves compounds belong to the class of Frank – Kasper phases showing topologically close-packed structures. They are categorized primarily into three parent members: the C14 hexagonal $MgZn_2$ type ($P6_3/mmc$), the C15 cubic $MgCu_2$ type ($Fd\text{-}3m$) and the C36 hexagonal $MgNi_2$ type structures ($P6_3/mmc$).

The discussion on the special properties of Laves phases started in the 1920s and 1930s. Laves work gave the first valuable insight into the characteristics of this class of materials. Especially in the last 30 years AB_2 type Laves phase compounds have been a subject of particular interest in solid state physics due to the variety of their physical properties. Today, over a thousand binary and ternary Laves phase intermetallics have been synthesized and characterized, of which about 60% contain a rare earth metal atom.

Motivated by describing the Os-based Laves superconductors, we synthesized and tested $R\mathrm{Os}_2$ materials (R = Lu, Y, Sc). The bulk nature of the superconducting transitions for $LuOs_2$, YOs_2, and $ScOs_2$ is evident from the visible anomalies at T_c = 3.47 K, 4.55, and 5.36 K, respectively.

The heat capacity experiment revealed that all compounds are moderately coupled type-II superconductors.

The work at GUT was supported by the National Science Center (Poland), project No.2019/33/N/ST5/01496.

Poster PS-10

Crystal growth and physical properties of TbM_2Al_{20} (M=Ti, V, Cr)

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The whole family of RM_2Al_{20} compounds of $CeCr_2Al_{20}$ type of crystal structure (space group No. 227) is attracting attention due to interesting physical properties like heavy fermion behaviour, Kondo effect [1], and various magnetic properties. It is all connected with its interesting crystal structure, where Al forms cages with rare earth R atom sitting inside, while transition metal M forms system of tetrahedra around.

Here the single crystal $TbTi_2Al_{20}$, TbV_2Al_{20} and $TbCr_2Al_{20}$ have been prepared by the Al self-flux method from the starting elements Tb, Ti/V/Cr and Al in the atomic ratio 1:2:90. The crystal structure has been characterized using powder x-ray diffraction and the $CeCr_2Al_{20}$ type has been confirmed. We discuss the physical properties of these compounds on the basis of measurements of magnetization, heat capacity, and electrical resistivity.

This work was supported by the National Science Centre (Poland), Grants No. 2017/26/E/ST3/00119 (B.W. and S.G.).. S.G. was also partly supported by the EU Project No. POWR.03.02.00-00-I004/16

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Poster PS-11

The impact of metal atoms diffusion on thermal decomposition of $In_xGa_{1-x}N$/GaN MQWs – first principles calculations

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In the last decade InGaN/GaN multi-quantum wells (MQWs) applied in Light Emitting Diodes (LEDs) and Laser Diodes (LD) have found many applications in illumination technology, medicine or environmental protection. It is well known that the structural quality of $In_xGa_{1-x}N$/GaN active regions, i.e. compositional homogeneity of MQWs as well as their interfacial morphology, have a significant impact on the device performance. A relatively low growth temperature is required for appropriate incorporation of In atoms into $In_xGa_{1-x}N$ layers. However, it can cause a reduction in the surface mobility of atoms and promote formation of point and extended defects. Additionaly, high In-content $In_xGa_{1-x}N$ layers exhibit a tendency to degrade when exposed to high temperatures. As reported by several authors, the critical temperature triggering thermal degradation of $In_xGa_{1-x}N$/GaN MQWs decreases with increasing In-content [1,2]. In order to get insight into the mechanism of thermal degradation of $In_xGa_{1-x}N$/GaN MQWs we performed DFT-based calculations aiming at the determination of the unknown diffusion coefficients D_{Me} of metal atoms in the $In_xGa_{1-x}N$/GaN structures with various In concentration (x = 0, 0.11, 0.22).
We used a supercell model of $In_xGa_{1-x}N$ alloys, either with the size of 3×3×3 or 9×9×3. The first supercell's size was used to calculate the heights of the migration energy barriers of Ga and In atoms diffusing in $In_xGa_{1-x}N$ alloys via the vacancy mediated mechanism. The latter one was used to perform phononic calculations of $In_xGa_{1-x}N$ system in harmonic approximation. In particular, we found the vibrational frequencies of $In_xGa_{1-x}N$ alloys in the presence of migrating point defects, and next, using the harmonic transition state theory, we found the temperature dependencies of the attempt frequencies of Ga and In atoms migrating in $In_xGa_{1-x}N$ systems, as well as their diffusion coefficients; D_{Ga}, D_{In}.
The obtained results show a significant decrease in the height of the migration energy barriers of In atoms in $In_xGa_{1-x}N$ alloys from 2.10 eV to 1.37 eV with the increase of In concentration from 0 to 22%. The corresponding heights of the migration energy barriers of Ga atoms in the same systems remains practically the same, and is of the order of ~2.75 eV. This indicates a possible higher diffusion of In atoms as compared to Ga atoms in $In_xGa_{1-x}N$ alloys. This statement is confirmed by the calculated temperature dependencies of diffusion coefficients of D_{In} and D_{Ga} in $In_xGa_{1-x}N$ alloys. Both In and Ga atoms are more mobile in $In_xGa_{1-x}N$ alloys than in bulk GaN. Moreover, In atoms diffuse faster than Ga atoms both in $In_xGa_{1-x}N$ alloys and in GaN. For example, D_{In} ($In_{0.22}Ga_{0.78}N$) at 800 ^{0}C is 8.75×10^{-12} cm^{2}s^{-1}, whereas D_{Ga} ($In_{0.22}Ga_{0.78}N$) at the same temperature is 6.47×10^{-17} cm^{2}s^{-1}. We show that as a consequence of the unbalanced diffusion rates of metal atoms between the $In_xGa_{1-x}N$ and GaN materials, some vacancies can be introduced to the interfacial area of $In_xGa_{1-x}N$/GaN QW, whose accumulation can be one of the main reasons for the thermal decomposition of $In_xGa_{1-x}N$/GaN MQWs system.

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Poster PS-12

Synthesis and Characterization of the solid solution series $NaYb_{1-x}Lu_xS_2$ in the α-$NaFeO_2$ structure type

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Materials with the α-$NaFeO_2$ structure have lately attracted considerable interest in quest of a unique magnetic ground state – the quantum spin liquid (QSL) state. In this structure type antiferromagnetically interacting trivalent rare earth ions with $J_{eff} = ½$ can be arranged on a regular triangular sublattice (see Figure 2) thus providing the perfect geometrical basis to study this kind of frustrated spin system. Indeed, no magnetic order was found in $NaYbCh_2$ (Ch = S, Se) down to 260 mK[1,2].

To investigate the interplay of the electron spins with respect to the magnetic properties in detail, we subsituted the Yb^{3+} ions in $NaYbS_2$ with non magnetic Lu^{3+} to dilute the magnetic sublattice. As the spin-spin interactions are influenced by the geometric confinements of the structure we had a detailed look on the structural parameters before determining the magnetic susceptibility and the electron spin resonance (ESR) properties. We characterized the samples of the solid solution series $NaYb_{1-x}Lu_xS_2$ with $0 \leq x \leq 1$ with respect to their chemical composition, analyzed their structural parameters in single crystal and powder X-ray diffraction experiments and evaluated the structural changes (see Figure 1 for the lattice parameters) throughout the whole substitution series.

We acknowledge support by the Deutsche Forschingsgemeinschaft via CRC 1143 (project-id 247310070).

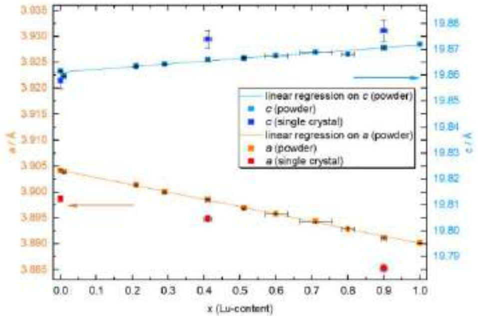

Figure 3: Refined lattice parameters of $NaYb_{1-x}Lu_xS_2$ samples derived from powder and single crystal data.

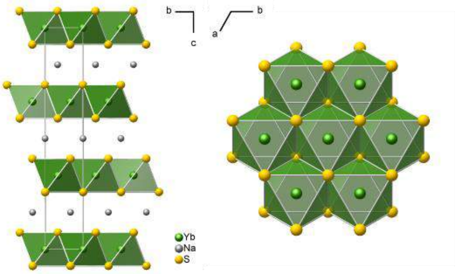

Figure 2: Crystal structure of $NaYbS_2$ in $R\bar{3}m$.

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Poster PS-13

ZnTe and CdTe layers as a contact for the high-resistivity (Cd,Mn)Te crystals

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High resistivity (Cd,Mn)Te is X and gamma-ray detector material. The II-VI semiconductors with resistivity above 10^9 Ωcm suffer from the ohmic contacting problem due to their high electron affinity and relatively large work function compering to metals. To solve the problem of work function mismatch an amorphous layer as a semiconductor and metal junction was proposed by Sebestyen [1]. Such layers with a high density of defects provide better charge transport between metal and semiconductor material.

We believe that due amorphous layer of ZnTe or CdTe, it is possible to equalize the Fermi levels between (Cd,Mn)Te and metal. Our previous works showed linear I-V characteristics obtained on monocrystalline and amorphous ZnTe layers heavily dopped for p-type with Sb and covered by Au [2].

We will present our recent results obtained from (Cd,Mn)Te samples with resistivity in the range 10^9-10^{10} Ωcm. In this work, we want to focus on amorphous/polycrystalline layers. ZnTe, ZnTe:Sb, ZnTe:In, CdTe and (Cd,Mg)Te layers were deposited in MBE chamber and covered by AuPd layer. Contact properties measurements, as well as SEM and TEM observations, will be presented.

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Poster PS-14

Effect of different pulling rates values on photoelectrochemical response and stability of $SrTiO_3$-TiO_2 photoanodes

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The idea of employing sunlight – virtually inexhaustible source of energy, in order to catalyze various chemical reactions or generate electrical current is intensively studied nowadays. Hydrogen is considered a promising energy source, especially when produced by direct conversion of solar energy in so-called photoelectrochemical cels (PEC). The possibility of considering versalite combinations of various component materials in eutectics provides a broad palette for many applications [1-3]. Eutectics obtained by the self-organization mechanism seems to be very attractive as energy-generating materials. They have potential as photoactive materials, due to their multiphase character – various available photoactive phases, multiple band gap energies and high crystallinity. The last research on the eutectic composites [4], [5] obtained by m-PD method confirmed that eutectic systems can be suitable for photoelectrochemical hydrogen production.

The aim of this work is to show the effect of using diferret pulling rates during growth process in $SrTiO_3$-TiO_2 eutectic composite applied as an active photoanode material for PEC. The characterization of the eutectic layers will be presented together with the photoelectrochemical measurements performed on fabricated photoanodes.

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Poster PS-15

Electrochemical reactions in thermogalvanic cells based on ionic liquids supplemented with iron oxide particles.

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Thermogalvanic cells work on the principle of the thermoelectric effect (Emiliano Bilotti, 2018) (Champier, 2017). Here, we investigate the behaviour of $(Fe_2O_3)_{n=1,2,3,4}$ particles in an ionic liquid (IL) environment and additionally in the presence of citrate ions. In detail, the structures are optimised at the density functional theory (DFT) level using the unrestricted open-shell wave function for the Becke3LYP hybrid correlation functional with an ECP basis set, denoted as UB3LYP/SBKJC. For all optimal spin and space configurations, we computed the standard redox potentials of the one-electron oxidation reactions using an adapted Born-Haber cycle scheme (Fig. 1).

In short, it reveals that the presence of the surrounding ions of the ILs leads to strong interactions of Fe^{3+} ions of the nanoparticle with the electronegative fluorine atoms of tetrafluoroborate anions irrespective of the size of the system in question. Almost always, the highest spin states correspond to the most stable structures. Ionic liquid cations are involved in the formation of hydrogen bonds between the oxygen ions of ferromagnetic nanoparticles and hydrogens of the cations. The standard redox potential of the one-electron oxidation reaction of our ferrofluid is almost the same as the standard redox potential obtained for neat iron (III) oxides. This indicates the redox process remains unchanged when the ferromagnetic nanoparticles are in ionic liquid systems, which can constitute strong bonds. In this case, Fe^{3+} ions are directly involved in the one-electron redox reaction. Consequently, the singly occupied orbitals are involved in the redox process.

$$\begin{tikzcd}
(Fe_2O_3)_n^{''}{}_{(g)} \arrow[r, "\Delta G_{ox}(g)"] \arrow[d, "\Delta G^{II}_{solv}"'] & (Fe_2O_3)_n^{'}{}_{(g)} \arrow[d, "\Delta G^{III}_{solv}"] \\
(Fe_2O_3)_n^{''}{}_{(aq)} \arrow[r, "\Delta G_{ox}(aq)"'] & (Fe_2O_3)_n^{'}{}_{(aq)}
\end{tikzcd}$$

Fig.1 Born-Haber cycle of the oxidation reaction.

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Poster PS-16

Anisotropic V_2O_5-crystal growth in the driven systems

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Classic macroscopic monocrystal growth typically needs quasistatic conditions with low supersaturation. We discuss the opposite case of driven systems [1] – when intensive stirring of aqueous powder suspensions leads not only to large supersaturations, to very fast mass-transfer, but as well to additional, "ballistic", anisotropic erosion of various facets. In such cases one observes the relatively fast formation of anisotropic nanostructures – nanorods, nanobelts, nanodiscs [2, 3]. To obtain the phenomenological description of such situation, we follow the concept of ballistic events, introduced by G.Martin et al [1] for description of phase and structural transformations induced by radiation and ball milling. We introduce an additional ballistic term to kinetic equations for the growth of individual facets under the condition of intensive stirring. We demonstrate that in this case even relatively small anisotropy of attachment ability and ballistic detachment (erosion) may lead to very big anisotropy of the growing nanocrystals at the growth stage and especially at the ripening stage.
We realized our own version of the method of V_2O_5-nanobelts formation suggested in [2], and compared the kinetics of nanocrystal growth, of viscosity, pH and conductivity evolution at various stirring frequencies. Structural evolution of V_2O_5 powder in the water without stirring for long time (11 months) is also studied.

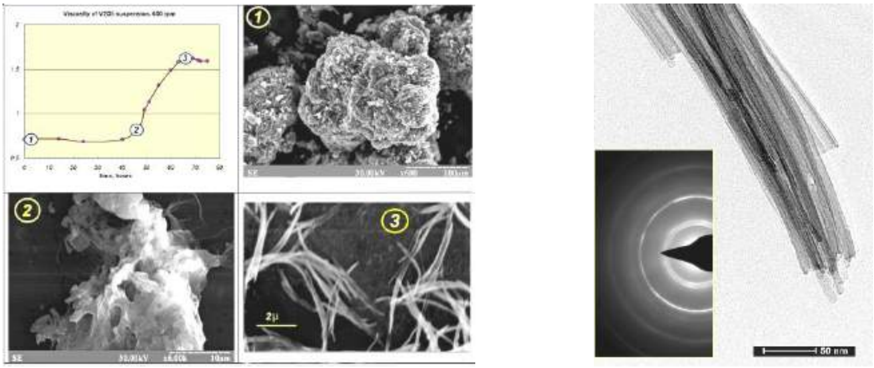

Fig.1 a) V_2O_5-crystal shape transformation; b) structure of nanocrystal

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Poster PS-17

Crystal growth of a ternary cage-like aluminide DyV_2Al_{20}

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The unique properties of solid materials often stem directly from their crystal structure. A prominent example of this relationship is a family of cage compounds that crystallize in the $CeCr_2Al_{20}$-type structure, presented in Fig.1 [1]. In such compounds, one type of atoms forms a cage, which is then filled with another atom. If the one confined inside the cage have a smaller size than the available space, one can observe a so-called rattling effect [2]. It is defined as local and anharmonic oscillation of the atom inside, characterized by an unusually large amplitude, which can lead to fascinating phenomena, including enhanced thermoelectric efficiency (oscillation scatters phonons without affecting the electrical conductivity) or existence of superconductivity, as coupling to the rattling phonon modes can enhance superconducting T_c [1].

Single crystals of DyV_2Al_{20} were grown by a flux (Al) growth technique. Dy pieces, V powder, and Al pellets, weighted in the 1:2:50 atomic ratio, were put together in an alumina crucible and capped with a second crucible, with a frit-disc placed in between to separate the flux from the crystals. The crucible set was placed in a quartz tube backfilled with Ar to limit the destructive effect of Al vapors acting upon Al_2O_3 crucible walls.

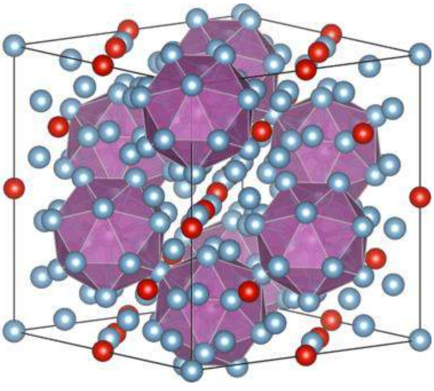

Fig.1 Crystal structure of $CeCr_2Al_{20}$-type intermetallics [1].

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Poster PS-18

Impact of the substrate on the efficiency of InGaN quantum wells

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InGaN quantum wells (QWs) are commonly used as the active region in light emitting diodes and lasers. In recent years, it has been shown that the performance of these devices can be degraded by the diffusion process of point defects (PDs). Such defects can accumulate in high-temperature (HT) n-type GaN layers during epitaxial growth [1]. Next, the PDs diffuse toward the active region and are captured by InGaN QWs to form non-radiative recombination centres, resulting in a significant decrease in the quantum efficiency of the QWs [2]. In the present study, we investigate whether a similar process can be induced by diffusion of PDs directly from a substrate. For this purpose, structures composed of a 500 nm HT GaN:Si layer and GaN/$In_{0.18}$GaN/GaN single QW were grown on a bulk GaN substrate and a standard GaN/sapphire template using the MOVPE technique. The effect of the substrate was investigated using cross-section cathodoluminescence measurements. Despite the use of a high-temperature GaN layer for both substrates, the QW emission was not detected only in the case of the bulk GaN substrate (compare Fig. 1a and c). Moreover, the wavelength-filtered image (Fig. 1b) showed that the near-band emission intensity of the HT layer decreases significantly close to the GaN substrate and only recovers at some distance from it. These observations suggest that both the HT epitaxial GaN layer and the SQW may be contaminated by point defects diffusing from the bulk GaN substrate.

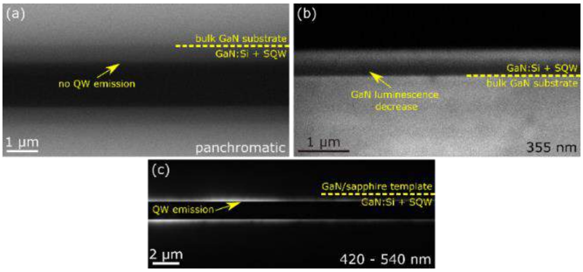

Fig.1 Cross-section cathodoluminescence images of the single quantum well (SQW) grown on (a and b) bulk GaN substrate and (c) GaN/sapphire template. (a) Panchromatic image indicating no luminescence detected from the SQW, (b) wavelength-filtered image showing decreased near-band GaN emission close to the bulk GaN substrate and (c) QW emission detected from the analogous SQW grown on the GaN/sapphire template.

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Poster PS-19

Influence of an excessive growth of crystalline phase on luminescence of phosphate glass - ceramics

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It is the need for new materials that forces us to look for unconventional solutions that, with a bit of luck, may turn out to be revolutionary. One of such steps was to propose glass - ceramics doped with rare earth elements as phosphors in LEDs. The coexisting crystalline phase produced in a controlled manner significantly improves the optical properties of the glass [1]. One of the obvious conditions for these materials is their transparency to visible light, which is achieved by limiting the growth of precipitated crystallites by selecting appropriate heat treatment parameters [2]. In this work, the conditions of a compromise between the transparency of the sample and the size of crystallites in the extreme case - leading to extensive surface crystallization of the glass - were investigated.

For the above purpose, 0.5 mol% europium doped phosphate glasses with the nominal composition $P_2O_5 – Bi_2O_3 – K_2O – Nb_2O_5 – SrF_2$ were subjected to two-stage annealing. In the first stage, the glasses were heated at 525°C for 10 hours. Two series were distinguished from the obtained samples, which were reheated for 22 hours in 545°C or 585°C, respectively. The acquired glass - ceramics were structurally characterized by XRD and FT-IR measurements. The effect of crystallization on Eu^{3+} ions luminescence was analyzed on the basis of the luminescence emission spectra under UV excitation.

Based on the research carried out, it was found that the excessive growth of the crystalline phase does not favorably affect the luminescence of europium ions embedded in glass - ceramics.

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Poster PS-20

Growth of UNi_2Si_2 single crystals and possible Lifshitz point in its magnetic phase diagram

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UNi_2Si_2 is a ternary silicide crystallizing with the tetragonal $ThCr_2Si_2$-type structure, which belongs to the intensively studied UT_2M_2 family (T = d-electron transition metal, M = Si, Ge). The compound shows complex magnetic properties [1,2]. In zero magnetic field, it undergoes a series of subsequent magnetic phase transitions from paramagnetic (PM) to incommensurate spin-density-wave (ICSDW) to simple body centered antiferromagnetic (AF), and eventually to ferrimagnetic (UAF) states. Application of external magnetic field causes metamagnetic transitions and stabilizes the UAF state. In high magnetic fields, PM, ICSDW and UAF phases tend to meet at a single point that may bear features of bicritical Lifshitz point (LP), which exibits critical behavior strikingly different from any other [3].
With the main aim to verify the LP hypothesis, we performed comprehensive reinvestigation of UNi_2Si_2 on high-quality single crystals grown using Czochralski pulling technique. Their quality was checked using EDS microanalysis, X-ray powder diffraction, and Laue diffraction method. The latter one was then used to determine crystallographic orientation of the sample. Physical properties of the compound were studied in the temperature range 2 – 300 K and in magnetic fields up to 14 T, aligned along the crystallographic c-axis that is the easy magnetic direction in the system. The results of our magnetic, electrical transport and heat capacity measurements confirmed the existence of multiple magnetic phases, and the tendency to merging the PM-ICLSW and ICLSW-UAF phase boundaries in the magnetic phase diagram constructed. However, up to 14 T, no clear evidence for Lifshitz point was obtained. Further detailed study of this interesting compound in stronger magnetic fields is indispensable.

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Poster PS-21

MBE-grow AlGaAs/GaAs QWIP for commercial production

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Quantum well infrared photodetectors (QWIPs) have a large industrial base with a number of military and commercial applications. Due to inter-subband transitions in the conduction band, the n-type QWIP detection mechanism requires photons with non-normal angle of incidence to provide proper polarization for photon absorption. The absorption quantum efficiency is relatively small, but the energy separation can be very well defined and tuned to the spectral range from ~ 3 µm to ~ 20 µm[1]. The GaAs layer thickness determines the well width, the Al% in the barrier AlGaAs controls the well depth. The proper geometry and the additional intentional doping by the Si can improve the quantum efficient. Du the fact that in such heterostructures the tight control is required over the material composition and layer thickness the Molecular Beam Epitaxy (MBE) growth technique is the preferred technique for growing the demanding QWIP structure. In this paper we demonstrate the 2 inches QWIP GaAs/AlGaAs heterostructures tuned for about 8um spectral range for dedicated for commercial use.

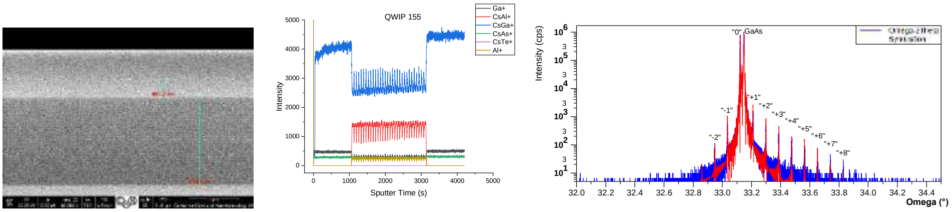

Fig.1 a) SEM image of the QWIP cross section; b) SIMS analysis of the QWIP structure; c) HRXRD results with simulation

We also present the results different kind of measurements such as the HRXRD, Raman and PL Spectroscopy, AFM, SIMS spectroscopy or SEM measurements the series of QWIP with: a) different geometrical ration (different width GaAs-quantum wells and AlGaAs-quantum barriers); b) different intentional doping QWIP obtained for series of different process made by MBE. These results are very important from the point of view of the commercial use which requires the homogeneity which should be over 98% of the all parameters for presented QWIP for the entire 2 inches surfaces. Our study allow to get the higher quantum efficient then in the similar QWIP structures presented in the literature.

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Poster PS-22

Control of lamellar growth in bismuth-based eutectic materials

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In this work, Bi_2Te_3-Te & Bi_2Te_3-BiTeI eutectic composites were obtained. The eutectics are the combinations of the minority phase of the topological insulator - Bi_2Te_3 and the majority phases, the Te or BiTeI semiconductors. The geometric sizes of the lamellas/layers, in the eutectic microstructure, depends on the growth conditions, i.e. the crystallization parameters [1,2]. In this work we studied the control of lamellae's dimensions and their numbers with the applied growth rate. We have varied the growth rates from 1.2 mm/h to 20 mm/h, which resulted in ~80µm to ~1µm width of the lamellae, respectively. A large number of parallel-to-each-other thin lamellae of the topological insulator increases the ratio of the surface state electrons to the electrons originating from the bulk. An atomically smooth interfaces between the two phases were created. Topological eutectic composite obtained in this way may overcome the challenges [3], currently preventing the widespread utilization of them.

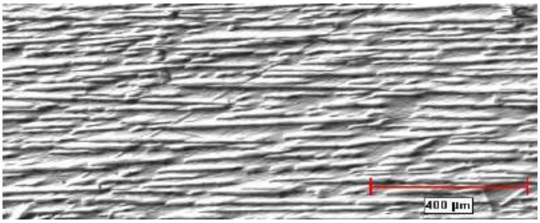

Fig.1 Pictures from an optical microscope. Visible thin lamellae of the Bi_2Te_3 topological insulator against the background of the tellurium (Te) matrix.

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Poster PS-23

Structural and luminescent properties of borate-bismuth glass and glass-ceramics doped with fluorides and Re^{3+} ions

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In recent years a lot of attention is focused on luminescent materials, due to the growing tendency to replacement traditional incandescent and fluorescent lamps with light-emitting diodes (LEDs). Especially, there is a high demand for finding new materials for phosphors doped with rare-earth ions (Re^{3+}), to replace the nowadays use of YAG: Ce^{3+} luminophore. To obtain good luminescent properties, Re^{3+} ions should be embedded in the appropriate host matrix. Such a matrix, should have properties like for example: good transparency in a wide frequency range and low phonons energy. Borate-bismuth glasses enriched with fluorides or nanocrystals, seem to meet these expectations. The luminesce enhancement due to the presence of AlF_3, as well as SrF_2 nanocrystals, was found in tellurium glasses [1,2].

Two types of borate-bismuth glass systems (B_2O_3-Bi_2O_3) modified by the addition of aluminum fluoride and strontium fluoride were successfully synthesized by conventional melt quenching technique as host matrices for optically active Eu^{3+}/Dy^{3+} ions. The strontium fluoride nanocrystals were prepared by heat-treatment process. The structure of obtained glass samples was characterized by XRD, DTA, and FTIR methods. The XPS analysis was conducted to obtain information about the valence states of elements present in glass samples. To examine the influence of fluorides addition on luminescence properties of borate-bismuth glass matrices were investigated by excitation under UV light. Additionally, CIE chromatic coordinates diagrams were calculated to define the colors emitted by samples doped with Eu^{3+}/Dy^{3+} in different molar ratios.

The results show that proposed materials seem to be appropriate matrices for rare-earth ions addition. Moreover, they can be considered as phosphors for light-emitting diodes (LEDs) applications.

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Poster PS-24

Control of magnetocaloric properties of $Gd_{7-x}Y_xPd_3$ (1 ≤ x ≤ 5) system by microstructure modification

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The $Gd_{7-x}Y_xPd_3$ (1 ≤ x ≤ 5) alloys were synthesized in various forms and structural states by the Czochralski growth from a levitating melt, vacuum suction and melt-spinning in order to investigate the effect of microstructure on the magnetic and magnetocaloric properties. Structural investigations were carried out using X-ray diffraction, while the microstructure was studied utilizing scanning electron microscopy. The magnetic and magnetocaloric properties clearly depend on the grain size and structural disorder. With increasing of the Y-content, the ferromagnetic transition shifts down to lower temperatures, namely whereas Gd_6YPd_3 single crystal orders ferromagnetically below 299 K, $Gd_5Y_2Pd_3$, $Gd_4Y_3Pd_3$, $Gd_3Y_4Pd_3$ and $Gd_2Y_5Pd_3$ single crystals undergo the magnetic transformation at 263 K, 240 K, 197 K and 144 K, respectively. The $Gd_{7-x}Y_xPd_3$ alloys in the form of rapidly cooled cast exhibit the magnetic transition temperatures at 305 K, 262 K, 242 K, 202 K and 153 K, for (1 ≤ x ≤ 5) respectively. The Curie temperatures of melt-spun $Gd_{7-x}Y_xPd_3$ alloys are much lower compared to rc-cast samples. The melt-spun Gd_6YPd_3 orders ferromagnetically below 115 K, while $Gd_5Y_2Pd_3$, $Gd_4Y_3Pd_3$, $Gd_3Y_4Pd_3$ and $Gd_2Y_5Pd_3$ ribbons undergo the magnetic transformation at 90 K, 65 K, 40 K and 25 K, respectively. Ribbons exhibit almost doubled magnetic entropy change in comparison to rc-cast samples. For instance, the $-\Delta S_m$ value for single crystal, melt-spun and rc-cast $Gd_5Y_2Pd_3$ is equal to 4.22 $Jkg^{-1}K^{-1}$, 6.31 $Jkg^{-1}K^{-1}$ and 3.64 $Jkg^{-1}K^{-1}$, respectively. Moreover, due to the large *FWHM* of the magnetic entropy change peak, the single crystals, melt-spun and rc-cast samples exhibit large refrigerant cooling power (*RCP*) comparable to those of some potential magnetic refrigerants.

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Poster PS-25

The influence of slip rate on the nature of distribution of microhardness of the surface layers of metal by depth

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Under friction conditions, the surface layers of metal are located within the influence of the complex stressed state, which is created by simultaneous action of normal and shearing stresses. In this case, the deformation of surface layers proceeds predominantly in the direction of action of shearing forces, which leads to texturing of surface layers, their hardening and work hardening. The hardening of the surface layer in active lubricating medium renders a screening effect for spreading the plasticity deformation into the depths of the metal [1]. The formation of the hardened surface layer prevents formation of particles of the wear and, therefore, decreases wear intensity.

The rollers made of steel 45 (HRC 38, Ra 0,57 microns) were used as the samples. The lubrication of contact surfaces was achieved by dipping the lower roller into a tray with oil. Mineral transmission oil for mechanical gearboxes and main drives of passenger cars and trucks Okko GL–4 80w/90 was used as the lubricant. The volumetric temperature of oil was 20o C. The maximum rotation frequency for the advancing surface amounted to 1000 r/min. The slippage 10 %, 20 %, 30 % and 40 % was imitated in the work. The maximum contact stress according to Hertz was 250 MPa.

With an increase in the slippage, the hardening of contact surfaces increases, which is a result of the increase in the deformation component of the friction coefficient with the increase in the slip rate from 0,315 m/s to 1,14 m/s at 10% and 40% slippage, respectively. The depth of spreading the stressed and deformed state of friction pairs depends directly on the degree of slippage of contact surfaces. For example, the depth of the amorphizated deformed layer of metal after etching (by the 4% alcohol solution of nitric acid) of the microsections of the lagging surface with the slippage 20% covers 30 – 37 µm, and with the slippage 40% – 100 – 300 µm.

In paper [2], a change in the physical and mechanical properties of the deformed contact surfaces of medium–carbon steel was found, with an increase in temperature at friction due to formation of secondary structures, oxide and higher oxide films.

With an increase in the slip rate from 0,315 m/s to 1,14 m/s at rolling with slippage, there was established an increase in the depth of spreading of the strained deformed state of contact surfaces as a result of the tribosystem transition to the boundary mode of lubricating action, which decreases the wear resistance of friction pairs.

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Poster PS-26

Structure redetermination, transport and thermal properties of the YNi_3Al_9 compound.

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The compounds RNi_3Al_9 (R=rare-earth metal Y, Gd, Tb, Dy, Er, Yb, Lu) attract attention because of their chiral polar structures, uncommon in general, possibly allowing for non-trivial spin textures. The structure of these compounds consists of alternating layers with compositions R_2Al_3, Ni, and Al. The closest R-R distances within R_2Al_3 layers are much shorter than corresponding distances between these layers causing 2D-like magnetic behavior, as the rare-earth metals are the only atoms with magnetic moment in the system. The comparison of compounds having non-magnetic atom (Y in the title compound, Lu) with ones hosting a magnetic rare-earth metals can help to study the electronic, lattice, and magnetic properties.

Single crystals of the YNi_3Al_9 compound were grown by self-flux method from the sample with initial composition Y:Ni:Al=1:3:20, having excess of aluminum. The obtained single crystals were several millimeters long with aspect ratio approx. 3:1. These results indicate possible existence of region on phase diagram, where the title compound is in equilibrium with liquid. Single crystal X-ray diffraction data clearly shows that the structure of the studied sample is completely ordered and belongs to $ErNi_3Al_9$ type, space group $R3_2$, a = 7.2838(2) Å, c = 27.4004(8) Å. Analysis of literature data on RNi_3Al_9 compounds shows clear trend towards formation of more ordered samples, while made by flux growth whereas formation of more disordered ones, while made by arc melting.

Electrical resistivity, magnetoresistance and heat capacity of the title compound were measured for the first time. It shows metallic behaviour with relatively high values of magnetoresistance up to 420% at low temperatures. The observed magnetoresistance can be explained by complicated Fermi surface, which was substantiated by the results of band structure calculations.

The heat capacity approaches the Dulong-Petit limit at high temperatures, while at the intermediate temperatures both dominating Debye and minor Einstein contributions to phonon heat capacity are observed. The calculated Debye temperature from low-temperature range θ_D = 566(5) K is significantly larger, than that from whole temperature range θ_D = 480(6) K and it is typical for aluminium-rich compounds. Corresponding Einstein temperature is θ_E = 198(8) K. The estimated value of electron-phonon coupling constant λ=0.092 suggests very weak coupling.

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Poster PS-27

Applying Photoelectron Spectroscopy to Study Surfaces

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Photoelectrochemical water splitting offers a sparkling and sustainable strategy for hydrogen generation, and significant research for enhancing the conversion efficiency of electrocatalysts is underway. Eutectic composite showed a great potential to create a highly stable and efficient PEC cell photoanode that can split water [1,2]. Despite the great potential of eutectic compounds in water splitting, there are missing systematic studies of the surface/interface of them exposed to water molecules using different electron spectroscopy methods. Such experiments can give a direct comparison with the surface/interface phenomenon and link them to the available application-oriented studies, providing the route to improve their properties.

Surface science emanated from the confluence of concepts and tools in physics and chemistry with technological innovations that made it possible to determine the structure and properties of surfaces and interfaces and the dynamics of chemical reactions at surfaces. The combination in the 1960s and 1970s of ultra-high-vacuum (i.e., $P < 10–7$ mbar) technology with the recognition that electrons in the energy range from 50 to 500 eV exhibited inelastic collision mean free paths of the order of a few angstroms fostered an explosion of activity. The results were a reformulation of the theory of electron solid scattering, the nearly universal use of electron spectroscopies for surface characterization, the rise of surface science as an independent interdisciplinary research area.

Applying eutectic compounds like $SrTiO_3$-TiO_2 as a substrate for single-layer graphene potentially can show outstanding results. Coupling TiO_2 with graphene has proven more active by photocatalysis than TiO_2 alone. It is generally considered that graphene sheets act as an electron acceptor facilitating the transfer and separation of photogenerated electrons during TiO_2 excitation, thereby reducing electron-hole recombination [3]. The concept of TiO_2 photocatalysis and how the interfacial charge transfer takes place between the TiO_2 and graphene to tune visible light activity, reduced annihilation of photogenerated charge carriers, and thereby its environmental implementations have been discussed in detail in reports [3]. However, methodologies and strategies to enhance the interfacial contact between TiO_2 and graphene in their hybrids like tailoring the exposed facets and morphology of TiO_2, defect engineering in TiO_2, functionalization, and doping in graphene nanosheets, are under investigation. Characterizations and understanding of the fundamental properties of such surfaces/interfaces extremely imply applying surface sensitive spectroscopies like X-ray photoelectron spectroscopy (XPS), near edge X-ray absorption fine structure (NEXAFS). In this regard, we will show how these techniques have been successfully applied to a similar system. Graphene grown on single-crystal metal surfaces offers ideal frameworks to investigate atomic level interactions in detail. In this poster, the hydrogenated graphene on a Pt-3d-Pt(111) subsurface alloys and corresponding graphene-metal interface have been investigated by means of temperature-programmed desorption (TPD), XPS, NEXAFS, and temperature-programmed XPS as an example, to show what kind of information we can extract from the surface [4,5] and we will apply the same procedure for Graphene/$SiTiO_3$-TiO_2 system.

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Poster PS-28

The analysis of casting stresses location in the root of single-crystalline Ni-based superalloy blades

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The nickel-based superalloys are the most widely used materials for production of turbine components, such as the blades, applicable in aerospace and energy sectors. Turbine blades are used in the most critical parts of aircraft engine, where an aggressive environment, high temperature and complex forces affect them [1].

Due to the specific dendrite structure of superalloys and complex shape of the blades, various growth defects, such as low-angle boundaries (LABs) [2], vacancies [3], and casting stress [4], may be formed during crystallization process. These root defects are inherited by airfoil during crystallisation of the blade and often do not disappear even after heat treatment is applied on production lines [4]. Therefore, even a small number of defects arising during crystallization may cause a decrease in strength properties [1]. Defects creation also cause a heterogeneity of dendrite structure. For this reason, it is important to analyse the as-cast structural heterogeneity of the blades.

The as-cast single-crystalline blades made of industrial nickel-based superalloy of CMSX-4 and CMSX-6 were studied. Single-crystalline turbine blades were produced by directional solidification using the Bridgman technique with a 3 mm/min withdrawal rate. The ALD Vacuum Technologies furnace in Research and Development Laboratory for Aerospace Materials, Rzeszów University of Technology was used. X-ray diffraction topography, the EFG W-scan X-ray diffraction method, scanning electron microscopy, and Laue diffraction were used to study the thin lamellar samples with a thickness of 0.5 mm and orientation of the surface perpendicular to the [001] direction.

Based on the results it was found that in the areas around the secondary dendrite arms, which grow toward each other to the collision, and around LABs, change in the lattice parameter of the γ'-phase occur. These lattice parameter changes are related to the internal stresses of the γ'-phase caused by local changes in the concentration of alloying elements and/or to the dendrite bending near the LABs. X-ray topography used on two surfaces of thin lamellar samples coupled with the lattice parameter measurements of the γ'-phase near the LAB allows separating the misorientation component of LAB diffraction contrast from the component and visualising the internal stresses of the γ'-phase.

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Poster PS-29

Efforts in searching for a efficient photocatalyst – sol-gel synthesis of vanadium pentoxide nanostructures with controllable morphology

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Water quality is one of the primary challenges that societies will face during the 21st century. According to UNESCO-IHP International Initiative on Water Quality, the availability of the world's water resources is increasingly limited due to the worsening pollution of freshwater. From the known methods of treating wastewaters, photocatalysis is a promising technology to solve environmental problems. Therefore, new and efficient photocatalysts that will be active in visible light and/or near-ultraviolet light, biologically neutral, photostable, and resistant to the influence of the environment are constantly being sought. Recently, vanadium pentoxide (V_2O_5) has received significant attention as a visible-light-driven photocatalytic material, owing to its slim bandgap energy of 2.40 eV, lower cost, and the two-dimensional layered structure [1]. The conducted research is focused on nanostructured vanadates because shape and size, as well as specific surface area, play a significant role in photocatalytic properties.

In the present work, we have focused on the synthesis and characterization of V_2O_5 nanostructures using the sol - gel method. The starting solution was prepared by mixing vanadium (V) oxytripropoxide in different solvents and condensation reagents. The bulk xerogel powders were annealed at 600 °C [2]. The vanadates' structural, morphological, and optical properties were characterized using different techniques such as XRD, FTIR, SEM, and UV-Vis DRS. Their photocatalytic activity was evaluated by the degradation of organic dye under simulated solar light illumination.

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Poster PS-30

Switching the optical properties of crystal-grown metamaterials

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Metamaterials with switchable optical properties are appealing for applications in fields as diverse as optoelectronics, optical sensors, or absorbers, among others. They display outstanding optical properties, which can be tuned dynamically and reversibly upon applying external solicitations, such as a temperature change, a voltage, a magnetic field, laser light, a deformation, changes in the chemical environment. A particular interest is currently focused on materials with switchable epsilon-near-zero (ENZ) properties, because they exhibit a number of unique features, such as the decoupling of spatial and temporal field variations, which enable the exploration of qualitatively different wave dynamics. ENZ materials bridge materials development and optical research. [1-2]

To develop real-world applications from switchable metamaterials, it is needed to produce such materials at a large-scale. Crystal-growth techniques, such as eutectic directional solidification, offer such possibility. $ZnO/ZnWO_4$ layered metamaterials grown by this method were used as outstanding temperature-controlled narrowband filters in the ultraviolet-blue region. [3] ZnO can also be doped, e.g. with Al, to endow the material with ENZ properties in the infrared. These properties can be tuned by varying the doping-induced carrier concentration and mobility, which control the plasma frequency. [4] Here, we further investigate the switchability of these materials under external solicitations, such as tempareture, a magnetic field, or an electrical excitation. In particular, we consider the use an external voltage, to tune this material in different wavelength regions.

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Poster PS-31

Single crystal growth of Eu-based topological materials using flux method

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The seminal discovery of topological insulators has ignited the development of intensive theoretical and experimental research on various classes of semiconducting and semimetallic materials with nontrivial electronic band structures. Recently, much attention has been paid to magnetic topological semimetals, which may harbor new exotic quantum states (e.g., chiral magnetic anomaly, large anomalous Hall effect) that can be used in practical applications such as spintronic devices. In this regard, Eu-based topological materials are particularly promising because Eu^{2+} ion bears a large spin-only magnetic moment.

In our on-going study, we focus at a family of ternary compounds with the chemical composition EuM_2X_2, where M = Zn, Cd, In, Sn, and X is a pnictogen. Single crystals of these materials can be synthesized using either self-flux or foreign-flux method. In this presentation, we will provide an overview of our attempts to obtain high quality crystals of sufficient size for a variety of thermodynamic and transport measurements, as well as for spectroscopic measurements. Optimization of growth conditions was routinely supported by examination of the chemical composition and crystal structure of the products by means of scanning electron microscopy combined with energy dispersive X-ray spectroscopy, as well as powder and single crystal X-ray diffraction.

Poster PS-32

Defect-structure characterization of $LaGaO_3$, $La_{0.88}Nd_{0.12}GaO_3$ and $SAT_{0.7}LA_{0.2}CAT_{0.1}$ single crystals

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Rare-earth containing oxides are important materials, dedicated e.g. for optoelectronic devices [1-3], fuel cells [4] or substrates applied to epitaxial growth of films and multilayers [5]. The present work is devoted to three different lanthanum-containing, Czochralski-grown single-crystal oxides: $LaGaO_3$, $La_{0.88}Nd_{0.12}GaO_3$ and $SAT_{0.7}LA_{0.2}CAT_{0.1}$ (where: SAT = $Sr_{0.5}Al_{0.5}TaO_3$, LA = $LaAlO_3$ and CAT = $CaAl_{0.5}Ta_{0.5}O_3$). All of the above mentioned crystals are perovskite-like but they represent various crystallographic systems: $LaGaO_3$ and $La_{0.88}Nd_{0.12}GaO_3$ are orthorhombic (Pbnm space group) [6, 7] and $SAT_{0.7}LA_{0.2}CAT_{0.1}$ is cubic (Fm-3m+Pm-3m space groups) [8].

The aims of the study were an analysis and a comparison of the samples' structural quality, important for the growth technology development. Experiments were performed by means of a high-resolution X-ray diffraction with a beam wavelength 1.5406 Å. The investigated samples had a form close to a cuboid with the largest surface size about 5 mm x 5 mm, (010)-oriented ($LaGaO_3$), (001)-oriented ($La_{0.88}Nd_{0.12}GaO_3$) and (110)-oriented ($SAT_{0.7}LA_{0.2}CAT_{0.1}$). Series of ω-scans at open detector (rocking curves), $2\vartheta/\omega$-scans and reciprocal lattice points maps were measured to assess an amount of extended defects in the investigated crystals and their chemical homogeneity.

The results show that the samples have a diverse crystal quality. In $LaGaO_3$ and $La_{0.88}Nd_{0.12}GaO_3$ crystal blocks and inhomogeneity of the chemical composition (due to the diversification of the lattice parameter *d* in the blocks) were detected. The blocks are misoriented up to 0.3° (in $La_{0.88}Nd_{0.12}GaO_3$). In $SAT_{0.7}LA_{0.2}CAT_{0.1}$ only micromosaics have been found.

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Poster PS-33

Influence of hight temeperature conducting interface on temperature induced fields in finite bimaterial solids

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This study considers development of analytic approach for studying temperature and temperature induced fields (mechanical, electric, magnetic) in pyroelectric/pyromagnetic bimaterial solids with coherent high temperature conducting interface, which often arise in analysis of modern composite smart materials, which are crystals in their nature [1]. Such coherent interfaces arise due to mutual penetration of materials on the interface and form a nanoscale layer with different properties, which can significantly affect thermal, electric and magnetic fields. The developed approach is based on the Stroh formalism and the least square approach. The Stroh complex functions are expanded in power series with unknown factors, and then boundary conditions are satisfied by the least square method, which allows determination of these unknowns. Thus, given the sought Stroh complex potentials, the problem is solved and all fields can be determined. This approach allows also to account for chemical potentials, which arise in crystal growth analysis, and another fields. Fig. 1 shows the temperature field in a square bimaterial solid with coherent imperfect interface, which can modell crystal growth on a substrate. It is visible that a little change in the interface heat conduction parameter µ0 significanlty influences temperature field in the substrate (and thus, other temperature induced fields), which can lead to technology induced defects. On the other hand, proposed approach can be used for development of appropriate technology of specific crystal growth on a substrate.

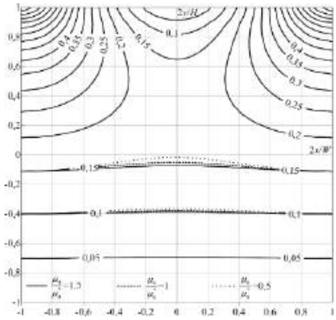

Fig.1 Temperature field in a finite bimaterial solid with high temperature conducting interface

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Poster PS-34

Physical properties of selected materials from $CaCoSi_nO_{2n+2}$ series

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Materials with general stoichiometry $CaCoSi_nO_{2n+2}$ are subject on several reports in a public space [1]. The best-known representative for n = 2 is pyroxene $CaCoSi_2O_6$ but not much is known about materials with n = 3 and n = 4 [2, 3]. In this study, attempts were carried out to synthesize those phantom materials and it was found that they do not exist as a single phase.

A quantitative XRD analysis revealed that their chemical composition is correct but the formula should be written as $CaCoSi_2O_6$ + (n-2)SiO_2. The X-ray Photoelectron Spectroscopy (XPS) and Si K edge X-ray Absorption Spectroscopy (XAS) techniques used respectively for electronic and magnetic (DC magnetometry) properties allowed to draw similar qualitative conclusions. Additionally, the DFT ab initio calculations were carried out to obtain electronic signature from band structure of $CaCoSi_2O_6$.

The apparent influence of the excess of SiO_2 on magnetic properties of this "series" can be understood in terms of presence and suppression of secondary phases like $Ca_2CoSi_2O_7$, which form when the starting materials are not homogenized properly. The mentioned secondary phases formation was suppressed by addition of surplus SiO_2 leaving clear signature from $CaCoSi_2O_6$. Using proper techniques, it is also possible to synthesized it from stoichiometric mixture.

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Poster PS-35

Influence of mechanical treatment of (Cd,Zn)Te bulk crystals on the surface quality and optical properties

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CdTe-based crystals are prominent semiconductors that are considered to be one of the better materials for X-ray and gamma-ray detectors and in the active layers of thin-film solar cells. They are usually prepared as bulk crystals grown by some variation of Bridgman, travelling heating or vertical gradient freeze methods. This study is devoted to the collection of crystals obtained with the addition of 3-4 at.% of zinc, which is believed to substitute between 6 and 8% of isoelectronic, but larger, cadmium atoms to improve the mechanical properties and to increase the bandgap of the obtained material.

The aim of this work was to investigate the influence of mechanical treatment of (Cd,Zn)Te bulk crystals on the surface quality and their optical properties using spectroscopic ellipsometry, radioluminescence, transmittance and Raman spectroscopy, as well as FTIR measurements. Our research has shown how individual steps of mechanical treatment of crystals and how different etching solutions affect their surface and optical properties.

Poster PS-36

{ZnO/MgO} superlattices grown on *a*-polar ZnO substrates by MBE – structural and optical studies

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Zinc oxide is intensively studied as a potential multi-functional material alternative to GaN. It is due to the wide bandgap, stable excitonic emission up to room temperature due to large exciton binding energy, and ease of alloying with group 2 elements such as Mg or Cd. Proper control of the energy gap in {ZnO/MgO} superlattices (SLs) can give a chance to obtain an active material in light-emitting devices.

The {ZnO/MgO}30 SL series with ZnO quantum well thicknesses from 1 nm to 2.5 nm and MgO quantum barrier from 1 nm to 3 nm were grown by plasma-assisted MBE. ZnO substrates were oriented in a-polar direction and were annealed at 650ºC prior to the growth process. Next low temperature ZnO buffer layers were grown. At the end the superlattice structures were grown at 550ºC.

The structural properties of the SLs were investigated by the high resolution X-ray diffraction (HR-XRD) and the characteristic satellite lines surrounding the main peaks, coming from the periodic structure of SLs, were clearly observed (Fig. 1a). X'Pert Epitaxy software based on the dynamical theory of X-ray diffraction and MROX code were used to simulate the obtained XRD data. The sublayer thicknesses of ZnO and MgO and strain relations in SLs were determined using XRD data simulations. The crystallographic quality of the SLs were analyzed with high resolution electron microscopy (HRTEM) (Fig. 1b). The rows of atoms are perfectly ordered in ZnO and MgO layers. The biaxial strains located mainly at the ZnO/MgO interfaces may cause eventual collation of the single crystallinity in the quasi-ternary alloys [1].

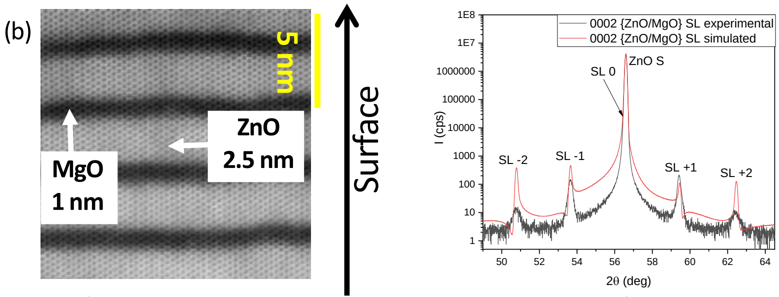

Fig.1 (a) 2θ/ω symmetrical XRD scan of 0002 reflection of {ZnO/MgO} SLs. (b) HRTEM analysis of {ZnO/MgO} SL structure.

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Poster PS-37

Strain distribution in GaN/AlN superlattices grown on AlN/sapphire templates: comparison of X-ray diffraction and photoluminescence studies

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GaN/AlN quantum structures are thoroughly studied because of a wide variety of their applications in light emitting diodes (LEDs) [1], photodetectors [2], solar-cells [3], etc.

Series of binary GaN/AlN superlattices with the same thicknesses of GaN wells and AlN barriers have been investigated. X-ray diffraction, photoluminescence and transmission electron microscopy techniques were used to study influence of the thickness of superlattice period on strain distribution in GaN/AlN multi quantum well (MQW) structures. Detailed X-ray diffraction (XRD) measurements demonstrate that the strain occurring in superlattices generally decreases with an increasing of well/barrier thickness.

Based on dynamical theory of X-ray diffraction the simulations of XRD curves have been performed. Fitting of XRD curves allowed to determine thicknesses of the GaN wells and of AlN barriers as well as the quality of the interfaces. The blurring of the interfaces causes deviations between experimental and calculated data. TEM measurements manifested the high quality of the interfaces in MQWs. For the samples with thinner wells/barriers the pin-holes and threading dislocations have been observed in TEM measurements. The best quality of interfaces has been registered for sample with well/barrier thickness of 3 nm. Finally, PL spectra showed that due to Quantum-Confined Stark Effect (QCSE) the PL peak energies of the MQWs decreased with increasing of the width of the GaN quantum wells and AlN quantum barriers.

The effect is reasonably well modelled by the *ab initio* calculations based on the density functional theory applied for tetragonally strained structures of the same geometry using a full tensorial representation of the strain in the MQWs [4].

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Poster PS-38

Synthesis and properties of selected transition metal phosphate magnets

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Transition metal [TM] (oxo)phosphates show a rich diversity of crystal structures and magnetic properties, arising from the interplay of local coordination, chemical bonding, and magnetic exchange interactions.

Here we present the results of our investigations on several TM phosphate compounds including ATMPO$_4$ (A – alkali metals; TM = Co, Ni, Cu), (AX)Cu$_5$O$_2$(PO$_4$)$_2$ (A – alkali metals, X – halides), and $Cu_{3+n}O_n(PO_4)_2$ (n =1,2).

The latter system shows signatures of low dimensional Cu^{2+} magnetism, despite the 3-dimensional character of the crystal structure. This stems from the quasi-one-dimensional superexchange pathway.

The (AX)Cu$_5$O$_2$(PO$_4$)$_2$ compounds feature a kagomé-related Cu^{2+} network and show sign of magnetic frustration that is partially relieved by structural distortion observed on cooling.

The ATMPO$_4$ group shows a variety of crystal structure types, ranging from a layered 2D found in $CsCuPO_4$ to a 3D zeolite-like framework of $RbNiPO_4$. In some cases, including $KCoPO_4$ and $KZnPO_4$ multiple different crystallographic phases can be obtained by modifying the synthesis route. Our results suggest the presence of magnetic frustration in the hexagonal chiral polar α-$KCoPO_4$ phase, which is absent in the orthorhombic δ-$KCoPO_4$ phase, despite structural similarities.

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Poster PS-39

In Vitro Dissolution of Na-Ca-P-Oxynitride glasses and glass-ceramics

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Na-Ca-P-O glasses and glass-ceramic composites doped with Mg and/or Si_3N_4 were synthesized. The results suggested that nitrogen was incorporated in the network of the homogeneous glasses and glass-ceramics. The glass-ceramics had high niobium content (up to 1.8 at%), and they consisted of calcium and sodium phosphate nanocrystallites and hydroxyapatite (HAp). The presence of HAp implied that these glass-ceramics might possess bioactive properties and thus be alternatives to the well-known bioactive phosphate glasses [1].
Accordingly, the *in vitro* dissolution of HAp-containing oxynitride glasses and glass-ceramics was investigated in SBF under static conditions up to 7 days. In all series, the release of Ca^{2+} from SBF was observed after immersion in the solution, indicating the HAp precipitation on samples' surfaces. The highest ions (Ca^{2+}, Mg^{2+}) release from SBF and ions (P^{5+}, Si^{4+}) release from samples' surfaces into SBF was observed at the initial stage of immersion (first day). The N incorporation into glass phosphate structure decreased its mean % mass loss at the early step of degradation, but improved its chemical durability through increased network connectivity. Furthermore, the incorporation of N remarkably affected *in vitro* dissolution of glasses compared to glass-ceramics. The results showed that the niobate incorporation increased the mean % mass loss of bioactive glasses and glass-ceramics. Moreover, no correlation was found between the pH changes and niobate contents. The calcium and sodium phosphates crystallites advanced the beginning of in vitro dissolution in glass-ceramics [1].

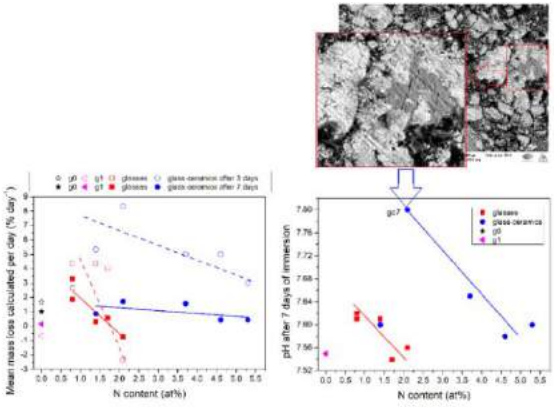

Fig.1 (a) Mean % mass loss calculated per day and (b) pH values after 7 days of immersion as a function of nitrogen content for glasses and glass-ceramics. SEM micrographs show the enlarged phosphates structures observed for sample gc7.

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Poster PS-40

Self-assembled growth of GaN nanowires on metallic ZrN nucleation layers for novel device applications

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The majority of results on nitride semiconductor nanowire (NW) growth by plasma-assisted MBE (PAMBE) were obtained on silicon substrates. However, in photonic devices using NW arrays on Si a large part of the light is lost by its absorption in the substrate. Moreover, the non-linear electrical Si/SiN_x/GaN junction inevitably forms at the bottom of the NWs that hinders carrier transport and heat dissipation near the NW/Si interface. Thus, there is a search for new substrates suitable for NW devices and the use of metallic nucleation layers is considered promising. Creating single-crystalline GaN NWs on metallic foils or films (Ti, Mo) has been reported already [1, 2]. However, it is known that Ga reacts with elemental metals leading to surface roughening and has detrimental effect on NW orientation and luminescence [3].

To avoid problems discussed above, instead of elemental metals we focus on metallic nitrides which are chemically stable and are easily deposited on various substrates by sputtering. In this work, we report on PAMBE growth of GaN NWs on Si substrates with 20 nm thick ZrN metallic buffers. AFM studies confirmed very smooth surface of the buffer (RMS = 0.58 nm for 10 µm × 10 µm scan) while transmission line measurements showed its low electrical resistivity of 1×10^{-3} Ωcm. XRD showed that ZrN films are polycrystalline with an average grain size of ~15 nm. Importantly, these values did not change after a long annealing in N flux at the NW growth temperature. Time-resolved PL measurements at 4K confirmed very high optical quality of the NWs, with narrow FX and D^oX lines. The I-V characteristics of the GaN NWs/ZrN system evidenced a low resistive ohmic contact to the bottom parts of NWs. Also a high optical reflectivity up to the UV range was measured on the NW-free edge of the wafer demonstrating that the ZrN buffer may act not only as the bottom electrode but also as a buried mirror reducing the light loses in NW based LEDs and photodetectors (photon recycling).

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Poster PS-41

Growth of Bi_2Te_3-Te and Sb_2Te_3-Te eutectic materials for thermoelectrics

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One of the promising and unconventional applications of eutectic materials are their use as thermoelectric materials. Materials based on Bi_2Te_3 and Sb_2Te_3 topological insulators create the best compounds that enable the conversion of low-parametric heat energy (up to 250°C) into electricity. In the micro/nano-scale eutectic heterostructural junctions, obtained by chemical synthesis or epitaxy give higher the figure of merit ($zT= S^2\sigma T/\kappa$) at room temperature [1,2,3]. Here, we present the thermoelectric parameters: thermal and electrical conductivity, Seebeck coefficient and dimensionless coefficient zT, in obtained eutectic and sub-eutectic bulk materials, which are based on Sb_2Te_3-Te and Bi_2Te_3-Te. The resulting interfaces at the two-phase boundaries are expected to contribute the scattering of inter-grain phonons, due to the lower thermal conductivity, which improves the thermoelectric zT coefficient. The obtained samples were characterized by Hall mesurmeants, Scanning Electron Microscopy (SEM), X-ray diffraction (XRD) and Energy Dispersive Spectroscopy (EDS). XRD measurements confirmed the phase purity and EDS shows chemical compostion of our samples.

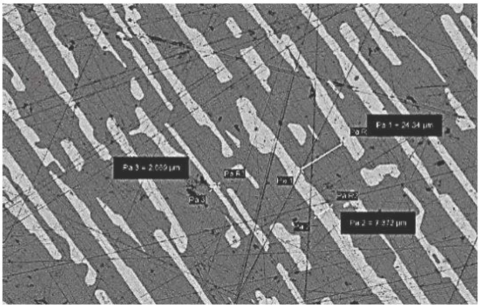

Fig.1 SEM image of Bi_2Te_3-Te eutectic structure, after Bridgman (VB) crystallization.

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