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Magnetic and Structural Studies of GeMnSnTe Epitaxial Layers

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GeMnTe is a multiferroic semiconductor, with interesting properties, such as coupling of ferroelectric and ferromagnetic orders, which results in ferroelectric domain switching under applied magnetic field. The latter can be observed with use of the ferromagnetic resonance (FMR) technique [1]. As interesting as GeMnTe is, its ferroelectric Curie temperature is considerably higher than the ferromagnetic one. Therefore, studying ferroelectric (rhombohedral) to paraelectric (cubic) phase transition in this system can not be investigated with use of the FMR technique. Co-doping with tin, however, has potential to lower the GeMnTe Curie temperature.

In order to study the effect of Sn co-doping on magnetic and structural properties of GeMnTe, $1\mu m$ thick Ge_{1-x-y}Mn_xSn_yTe layers were grown by MBE on (111) BaF₂ substrates, with Mn content x ranging from 10 to 30% and Sn content y ranging from 2 to 5%. Subsequently, the obtained layers were characterized with use of X-ray diffraction, atomic force microscopy, energy dispersive X-ray spectroscopy (EDX), and SQUID magnetometry. The magnetic anisotropy was studied with the FMR technique.



Fig. 1: FMR peak positions in $Ge_{0.85}Mn_{0.15}Te$ (left) and $Ge_{0.88}Mn_{0.1}Sn_{0.02}Te$ (right) layers vs. orientation of the applied magnetic field, at 3 and 10 K, respectively. The angle is measured from the [111] direction (c-axis) perpendicular to the layers.

Within the x and y ranges investigated all the layers were found at low temperatures ferromagnetic be to and rhombohedral, with the distortion axis perpendicular to the layer surface. As shown in Fig. 1, already co-doping with 2% changes considerably Sn the magnetocrystalline anisotropy: from purely uniaxial in GeMnTe (with 15% Mn) to distorted cubic in GeMnSnTe (10% Mn). The contribution of cubic anisotropy allows distinction of ferroelectric domains with rotated orientations of crystallographic axes. It was found, however, that tin co-doping results in only one domain orientation up to x = 27%, whereas in GeMnTe for x = 20% two such domains were observed. This suggests that domain switching in GeMnTe is probably related to magneto-elastic interactions, which are suppressed in Sn co-doped layers.

[1] H. Przybylińska, G. Springholz, R.T. Lechner, M. Hassan, M. Wegscheider, W. Jantsch, and G. Bauer, *Phys.Rev. Lett.* **112**, 047202 (2014).

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Ferromagnetic Properties of Topological Crystalline Insulator Sn_{1-x}Mn_xTe Layers on BaF₂ and GaAs Substrates

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Recent renewal of interest in SnTe-based IV-VI narrow gap semiconductors is due to the discovery of topological crystalline insulator (TCI) states at the (001) and (111) crystal surfaces [1,2]. In search for high quality TCI materials exhibiting both topological and ferromagnetic properties, we have grown a series of $Sn_{1-x}Mn_x$ Te layers with Mn content up to x = 0.08, deposited on various substrates: BaF_2 , with either (111) or (001) orientation and GaAs (001). In this work we compare the magnetic properties of these layers depending on Mn content and growth conditions.

Sn_{1-x}Mn_xTe layers of thickness in the range $0.25 - 1.5 \,\mu$ m were grown by molecular beam epitaxy (MBE). Magnetization measurements were carried out with use of a superconducting quantum interference device (SQUID), while for detailed magnetic anisotropy studies we applied the ferromagnetic resonance (FMR) technique. We found that the Sn_{1-x}Mn_xTe ($0.03 \le x \le 0.08$) layers with hole concentration $p > 2 \times 10^{20} \text{ cm}^{-3}$ grown on either substrate exhibit ferromagnetic behaviour at helium temperatures. In contrast, the layers grown in the regime of very low Te excess with relatively low carrier concentration ($p < 10^{20} \text{ cm}^{-3}$) remain paramagnetic down to 2 K. Even in the layers with the highest Mn content studied and hole concentration close to optimum, the ferromagnetic transition temperatures were below 10 K, i.e., about twice smaller than in bulk crystals [3]. In these layers the saturation magnetization observed amounts to about half of the expected value. It indicates that even in the optimal growth regime, the substitution of Mn ions at cation sites of the rock-salt lattice of SnTe is limited.

The analysis of the angular dependence of the FMR peak positions revealed a dominant shape anisotropy contribution for all investigated layers. However, while all (001) oriented layers were found to exhibit perfect cubic symmetry, those grown on BaF2 (111) substrates turned out to be rhombohedrally distorted along the [111] growth direction. Such a distortion is related to a ferroelectric phase transition. In contrast to $Ge_{1-x}Mn_xTe$ layers, where such crystal distortion induces perpendicular orientation of the easy magnetization axis [4], in $Sn_{1-x}Mn_xTe$ layers the easy direction of magnetization is located in the plane of the layer. Nevertheless, the coexistence of ferroelectricity, ferromagnetism, and TCI properties makes this system extremely attractive for investigations of the interplay among these three properties.

- [1] Y. Tanaka, Z. Ren, T. Sato et al., Nat. Phys. 8, 800 (2012),
- [2] K. Dybko, M. Szot, A. Szczerbakow et al., Phys. Rev. B 96, 205129 (2017),
- [3] P.J.T. Eggenkamp, H.J.M. Swagten, T. Story et al., Phys. Rev. B 51, 15250 (1995),

[4] H. Przybylińska, G. Springholz, R.T. Lechner et al., Phys. Rev. Lett. 112, 047202 (2014).

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Magnetoelastic, magnetic anisotropy and magnetic damping investigations of Cobased Heusler alloy thin films

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The series of half-metallic Co₂Fe_xMn_{1-x}Si (CFMS) Heusler alloys epitaxial thin films with the thickness of about 30 nm were investigated to determine the composition influence on magnetoelastic and damping properties and magnetic anisotropy. Magnetoelastic properties were examined by means of the Strain Modulated Ferromagnetic Resonance (SMFMR). Magnetic damping properties were studied by means of Vector Network Analyzer FMR (VNA FMR) which allows determining Gilbert damping parameter. Magnetocrystalline anisotropy was investigated by means SQUID and FMR techniques. Magnetoelastic constant as well as Gilbert damping factor dependencies versus magnetic layer composition were obtained. Magnetoelastic constant was found to be in the range 5-25 10^6 erg/cm³, with corresponding magnetostriction coefficient λ of about 6-30 10^{-6} , and Gilbert damping factor in the range 2-6 10⁻³. Correlations between the last two parameters were considered. Both parameters have small values, which is expected for CFMS magnetic layers as for representative of materials for both spintronic and magnonic applications. Magnetoelastic constants have similar values range as for Co₂Fe_{0.4}Mn_{0.6}Si thin films with thickness in the range 15-50 nm [1]. Gilbert damping factor has a minimum for composition x=0.4. This composition corresponds to the highest tunnel magnetoresistance ratio [2]. Except of this, there has been observed nonlinear behavior of FMR half maximum width ΔH versus frequency which has been previously observed for Co₂FeAl Heusler compound [3] and is attributed to the two magnon scattering by the line defect or dislocation networks.

- [1] O.M. Chumak et al, IEEE Trans. Magn. 53 2501906 (2017).
- [2] T. Kubota et al, Appl. Phys. Lett. 94 122504 (2009).
- [3] S. Mizukami et al, J. Appl. Phys. 105, 07D306 (2009).

Magnetic and magnetocaloric properties of Fe₇Se₈ single crystals doped with cobalt and nickel ions

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The main purpose of this research is to determine changes of magnetocaloric effect and spin reorientation phase transition in iron selenide Fe_7Se_8 (3c type) single crystals doped with 2% and 5% of cobalt ions, 2% and 10% of nickel ions. The single crystals have been grown using modified Bridgman's method. Magnetization measurements as a function of temperature and magnetic field have been carried out using magnetometer SQUID MPMS 7XL. It was shown that doping has important influence on both magnetocaloric effect and reorientation temperature. It has no effect on the crystal structure although it changes lattice parameters. Magnetocaloric effect related to the metamagnetic transitions has been found above the transition temperature while below this point inverse magnetocaloric effect was identified. Experimental results have been discussed in frames of the single ion model of the crystal field.

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Superconducting Properties of Iron Selenides Intercalated with Organic Molecules

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Layered iron selenides intercalated with organic molecules have attracted a lot of attention in the last few years. The magnetic and nonmagnetic mesoscopic phase separation in these materials opened discussion on the nature of superconducting phase and the role of organic intercalants in tuning of superconducting properties. Superconductors with general formula $(\text{Li-}O)_x(\text{FeSe}_zCh_{1-z})_y$ (O - Py, EDA; Ch - S, Te) were obtained by solvothermal intercalation of polycrystalline FeSe_z Ch_{1-z} using Schlenk technique. Magnetic measurements of their superconducting state properties have been performed by means of SQUID. Samples have been characterized by superconducting state transition temperature in the range 9 – 43 K, depending on their chemical composition. Relatively high transition temperature T_c around 43 K was shown by $(\text{Li-EDA})_y(\text{FeSe}_{0.88}S_{0.1})_x$. Upper critical field, H_{c2} , was determined with ac magnetic susceptibility in external magnetic field. It was found that H_{c2} , recorded in the temperature range up to 30 K, decreases with increasing temperature, with a coefficient dH_{c2}/dT typical for superconducting layered $A_x Fe_{2-y}Se_2$ (A = K, Rb, Cs). Importantly, the magnetic field range, where the superconductivity at the temperatures above 30 K is observed, corresponds to irreversibility field in the hysteresis loop. This may suggest that appearance of superconductivity at the temperatures higher than T_c of $A_x Fe_{2-y}Se_2$ is most likely related to magnetic inhomogeneity in the studied system.

Pockels Imaging in CdTe-based Compounds

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Due to a great importance of high energy radiation such as X-rays and gamma-rays in a wide range of applications including medical imaging, national security and basic science, in recent years there is a focus on developing semiconductor devices which can operate at room temperature [1]. In considered scope of radiation's energy (30-700 keV) electromagnetic wave interacts with a solid-state detector via photoelectric absorption mechanism [2]. Therefore in that group of detectors the leading materials are CdTe-based compounds – owing to their large cross-section for pondered radiation.

These materials should fulfill numerous requirements. One of them is a uniform distribution of internal electric field. This work presents results of examinations of (Cd,Mn)Te, (Cd,Mg)Te and (Cd,Mn)(Te,Se) crystals. In considered range of chemical composition, all mentioned materials crystallize in zinc blende structure so they do not have an inversion symmetry. Consequently it allows to make use of Pockels electro-optic effect in internal electric field investigations. It is observed when the angle of polarization of a linear polarized light beam is rotated after passing through the crystal under an applied electric field. When the crystal is placed between two crossed polarizers, the transmitted light intensity is a function of the internal electric field [3].

The Pockels image of sample with a uniform distribution of internal electric field should be of constant brightness (a constant value of refractive index in whole sample) what is desired. In (Cd,Mg)Te crystals, when IR light is perpendicular to the **(111)** direction, there are visible numerous parallel planes of twin boundaries which are decorated by spherical Te inclusions. In that region Pockels imaging has revealed an accumulation of charges. (Cd,Mn)(Te,Se) crystals contain both spherical line-formed Te and star-like isolated Cd inclusions. Despite the average size of Cd inclusion is bigger (~40 µm) than Te inclusion (~7 µm), there is no signal from it in Pockels imaging. Furthermore, the internal electric field measurements in such crystals are very difficult due to their low resistivity (ρ ~10⁵ Ω ·cm). The most promising material for a new nuclear detector is (Cd,Mn)Te because it is easier to achieve large-volume single crystals with much lower Te inclusions density (~5·10³ cm⁻³). As a result (Cd,Mn)Te samples often have a uniform internal electric field distribution.

- [1] T. E. Schlesinger et al., Materials Science and Engineering 32, 103 (2001),
- [2] A. Mycielski et al., Journal of Crystal Growth 491, 73 (2018),
- [3] M. Groza et al., Journal of Applied Physics 107, 023704 (2010).

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Epitaxial Growth, Structural and Electric Properties of SnTe/CdTe and Pb_{1-x}Sn_xTe/CdTe Topological Layers

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 $Pb_{1-x}Sn_xTe$ is a IV-VI narrow-gap semiconductor solid solution crystallizing in the rock-salt crystal structure with the lattice parameter varying from *a*=6.46 A for PbTe to *a*=6.32 A for SnTe and matching very well to zinc-blende II-VI semiconductor CdTe (*a*=6.48 A). Good lattice matching but different crystal structure and chemical bonding result in a variety of high quality nanostructures with atomically sharp interfaces observed, e.g. in related PbTe-CdTe materials system [1]. Recently, it was theoretically proposed that SnTe, $Pb_{1-x}Sn_xTe$ (x>0.4), and $Pb_{1-x}Sn_xSe(x=0.18-0.4)$ IV-VI crystals, known to possess inverted band ordering, are topological crystalline insulators (TCI). It is now confirmed with photoemission, scanning tunneling spectroscopy, and magnetotransport measurements of both bulk crystal and thin layers[2-6]. In contrast, CdTe is a semiconductor with topologically trivial band ordering. This materials system offers apossibility of preparing high crystal quality topological/trivial multilayers with relative contribution of topological interface states to the bulk of the crystalscontrolled by multilayer design.

A series of SnTe and Pb_{1-x}Sn_xTe layers (x=0.36 - 0.76) were grown by molecular beam epitaxy on GaAs(001) substrate with a very thick CdTebuffer. Thickness of the layers, varying from 0.2 µm to 3 µm, was measured with scanning electron microscope. By optimizing the temperature of growth and flux ratios of SnTe, Te, and Pb the optimal parameters were found for growing single-phase high crystal quality films.The deposition of films was monitored in situ by reflection high-energy electron diffraction to confirm the two-dimensional growth regime and crystal quality. The surface morphology was studied by atomic force microscopy revealing atomic steps and roughness parameter of 1.7 nm for 2x2 µm² region. The lattice parameter, strain, and degree of relaxation of SnTe layers were examined by high resolution X-ray diffraction method revealing, in particular, that SnTe layers are practically fully relaxed (relaxation degree about 96-98 %). An important physical parameter of SnTe and Pb_{1-x}Sn_xTe crystals is their non-stoichiometry that brings electrically active metal vacancies. We controlled this factor by Hall effect measurements revealing the expected very high conducting hole concentration of about $p=10^{20}$ cm⁻³, sensitive to excess Te growth regime.

- [1] M. Szot, K. Dybko, P. Dziawa et. al., Crystal Growth & Design 11, 4794 (2011),
- [2] P. Dziawa, B.J. Kowalski, K. Dybko et. al., Nature Mat. 11, 1023 (2012),
- [3] Y. Tanaka, Z. Ren, T. Sato et al., Nat. Phys. 8, 800 (2012),
- [4] S.-Y. Xu, C. Liu, N. Alidoust, M. Neupane et al., Nat. Commun. 3, 1192 (2012),
- [5] K. Dybko, M. Szot, A. Szczerbakow et al., Physical Review B 96, 205129 (2017),
- [6] V.V. Volobuev, P.S. Mandal, M. Galicka et al., Adv. Mater. 29, 1604185 (2017).

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Fabrication microdevices in epitaxially grown CdTe quantum wells

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Low dimensional heterostructures based on cadmium telluride are intensively studied for possible applications in optoelectronics (due to its direct band gap and near infrared to visible emission) as well as in spintronics (current induced spin polarization and spin filtering). We present results of our research aiming at producing high mobility CdTe structures doped with either Iodine or Indium donors and technology of fabrication microdevices using electron beam lithography.

We grew a series of structures with different fluxes, flux ratio and various substrate temperatures. Reflection high-energy electron diffraction (RHEED) was used to determine a growth rate and evaluate smoothness of grown layers. The samples were post-growth characterized using (i) scanning electron microscopy - to confirm thickness and check the smoothness of grown surface; (ii) photoluminescence - to determinate energy gaps of different layers and their composition; (iii) electron transport measurements at helium temperatures - to determinate electron concentration and mobility.

We are working at two kind of devices focused at spin separation and filtration. One of them was prepared in CdTe quantum well modulation-doped with iodine up to carrier concentration of about 1.2×10^{12} cm⁻² for achieve high spin density. The samples with different width of microchannels were prepared for Kerr rotation measurements to observe spin accumulation near edge of the conducting channel. Second one was prepared in high mobility modulation doped CdMgTe quantum well. Nanoscale, H-shaped channel with deposited micro-magnet nearby was prepared for electron transport measurements to observe current splitting and spin separation caused by weak inhomogeneous magnetic field.

Topological States on Uneven PbSnSe Surfaces

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The solid solution $Pb_{1-x}Sn_xSe$ is known to belong to the topological crystalline insulator class, under the condition that its bulk band gap is inverted. At room temperature this is satisfied for 0.3 < x < 0.4. High symmetry surfaces of such crystal – e.g., (001), (110), (111) – host metallic states dispersing linearly around Dirac points, whose degeneracy is protected by mirror symmetries of the rock-salt type lattice [1, 2].

As the bulk band gap is located at four L points, four Dirac cones are expected to appear on the surface. However, at the (001) cleavage plane, two L valleys project onto the same \overline{X} point in the surface Brillouin zone, causing the two associated cones to hybridize through valley mixing. Thus, a "double Dirac cone structure" (DDCS) is formed, in which the degeneracy at \overline{X} is split by tens of meV, while the two protected crossings are shifted away from \overline{X} along the $\overline{X} - \overline{\Gamma}$ line [3]. Recently, it has been shown that such valley splitting is extremely sensitive to morphology of the surface, e.g., in presence of densely spaced odd-height atomic ridges collapses completely to a doubly-degenerate cone [4]. Also the 1D states along sparsely distributed odd-height atomic step edges have been shown to originate from the DDCS [5].

Combining both a basic qualitative understanding of these phenomena [4, 5] and numerical tightbinding results we derived a simple envelope function model which explains such mutability of states on (001) $Pb_{1-x}Sn_xSe$ surface, but is also easily generalized to similar systems. The aim of my talk will be to present the basic concepts of the above method in an accessible manner.

- [1] T. H. Hsieh et al., Nature Commun. 3, 982 (2012),
- [2] S. Safaei et al., Phys. Rev. B 88, 045305 (2013),
- [3] J. Liu et al., Phys. Rev. B 88, 241303(R) (2013),
- [4] C. Polley et al., ACS Nano 12, 617-626 (2018),
- [5] P. Sessi et al., Science 354, 1269-1273 (2016).

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Instability of Exciton-Polaritons System in Semimagnetic Semiconductor Microcavity

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We study the system of exciton-polaritons condensate in a semimagnetic semiconductor microcavity [1,2], described by the Complex Ginzburg-Landau equation with additional magnetic spin relaxation equation for magnetic ions. Similar system was considered in [1], and here we extend it by including external pumping and losses.

Circularly polarized condensate can self-localize due to the exchange coupling interaction between polaritons and magnetic ions. We calculate the diagram of stability of magnetic polarons due to various physical parameters, emphasizing the special role of polariton-magnetic ion coupling constant λ_M . The stability was determined both by numerical solution of the Complex Ginzburg-Landau equation and the linear Bogoliubov approximation. Surprisingly, limiting values of λ_M that determine the stability depend strongly on the derivate of the Brillouin function, but not on the magnetic spin relaxation time, see Fig. 1a. The dependence on temperature and coupling constant λ_M is shown in Fig. 1b.



Fig. 1: Diagrams of instability. Color scale represents the instability rate. Cyan color shows that system is stable (it is symbolically expressed by 0 on logarithmic scale). Crosses and circles in Fig. 1a represents respectively stable and unstable states derived in evolution simulations.

I. A. Shelykh, T. C. H. Liew and A. V. Kavokin, *Phys. Rev B* 80, 201306 (2009),
R. Mirek, M. Król, K. Lekenta, J.-G. Rousset, M. Nawrocki, M. Kulczykowski, M. Matuszewski, J. Szczytko, W. Pacuski, and B. Piętka, *Phys. Rev. B* 95, 085429 (2017),
P. Miętki, M. Matuszewski, *Phys. Rev. B* 96, 115310 (2017).

Effective Two-Mode Description of the Dynamics of Interacting Bosons Confined in a Double-Well Trap

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Typically, when the dynamics of a few bosons in a double-well potential is studied, one uses a twomode model which assumes that particles can occupy the lowest orbitals localized in the left or the right well. Consequently all excited orbitals are neglected. This traditional model is sufficient to describe the system for sufficiently deep wells and in a weakly interacting regime, i.e., where the interaction energy per particle is much smaller than the single-particle excitation energy. However, the model rapidly becomes inaccurate as the interparticle interaction strength grows, since couplings to higher bands become non-negligible [1].

In my presentation I will show that, even for quite strong interactions, the dynamical properties of the system can be recovered accurately in the framework of a two-mode description if appropriate effective modifications are made. We describe two different approaches to this problem.

In the first method [2], we describe the system in terms of a specific basis of effective wave functions, uniquely tailored to the problem under study. The basis modes are directly derived from the many-body Hamiltonian. The shapes of the resulting basis wave functions take into account the interaction-induced modifications of the natural orbitals. This effective model gives accurate predictions over a wider range of interactions than the traditional model.

The second method [3], which can be used if the number of particles is larger than two, involves extending the many-body Hamiltonian with effective three-body interaction terms. These terms effectively account for various corrections that arise from virtual transitions to excited energy states. Two such terms, an on-site three-body interaction and an interaction-induced single-particle tunneling, are sufficient to recover the exact dynamics with excellent accuracy.

- [2] J. Dobrzyniecki and T. Sowiński, Phys. Lett. A 382, 394 (2018),
- [3] J. Dobrzyniecki et al., Phys. Rev. A 97, 013609 (2018).

^[1] J. Dobrzyniecki and T. Sowiński, Eur. Phys. J. D 70, 83 (2016),

Comparison of optical properties of GaN/AlGaN quantum structures grown along polar (c-plane) and non-polar (*m*-plane) crystallographic directions

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The built-in electric field in polar III-nitride heterostructures is a consequence of the high piezoelectric and spontaneous polarization in these materials. The electric field is particularly intense in the GaN/AlGaN system, which is at the base of the development of GaN-based high electron mobility transistors, but can be deleterious for the fabrication of ultraviolet emitters. The polarization-induced electric field affects basic physical properties, it causes a large red shift of the photoluminescence and lowers quantum efficiency due to the quantum confined Stark effect. Non-polar heterostructures, i.e. structures where the heterointerfaces are perpendicular to the <0001> polar crystallographic axis, are free from such negative features. In this work, we present a theoretical and experimental study of the optical behaviour of polar and non-polar GaN/AlGaN quantum wells (QWs).

The absence of built-in electric field in non-polar QWs causes drastic differences in their basic optical properties (e.g. like photoluminescence (PL) peak energy and PL decay times) as compared with their polar counterparts. Furthermore, the absence of electric field reduces the localization potential at alloys fluctuations. Therefore, the S-shape behaviour of the PL peak energy with temperature, observed in polar GaN/AlGaN QWs, is weaker or even not present in non-polar samples [1]. On the other hand, the pressure behaviour of polar and non-polar QWs is completely different. In polar QWs, the pressure coefficients are highly reduced with respect to that of the GaN energy gap, which is due to the hydrostatic-pressure-induced increase of the piezoelectric field in quantum structures and to the nonlinear behaviour of the GaN band gap.

[1] T. Langer, H-G. Pietscher, F. A. Ketzer, H. Jönen, H. Bremers, U. Rossow, D. Menzel, A. Hangleiter, *Phys. Rev. B* **90**, 205302 (2014).

Down-conversion process in the Bi³⁺-Yb³⁺ co-doped oxides

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Down-converting materials allowing conversion of light from UV to near-IR range nowadays are widely studied from the point of view of possible enhancement of silicon solar cells. An ideal down-converting material allows to increase the efficiency of silicon solar cell from 32 to 37% [1]. For this purpose, luminescent materials doped with rare-earth ions are usually discussed. However, these materials have several drawbacks such as narrow lines of absorption in UV range and low absorption cross-section of the f-f transitions. Therefore, the luminescent materials deprived of these drawbacks are required. From this point of view broad-band materials co-doped with Bi³⁺ and Yb³⁺ ions looks very attractive because of the broad absorption of Bi³⁺ in UV range and the emission of Yb³⁺ exactly above the band gap of silicon. The Bi³⁺ ion is known as efficient sensitizer for rare-earth ions and the energy transfer from Bi³⁺ to Yb³⁺ has been demonstrated (see e.g. [2]). However, the mechanism of such energy transfer, possibly cooperative energy transfer from one Bi³⁺ ion to two Yb³⁺ ions, remains questionable.

Usually for estimating of the mechanism of the down-conversion process in such double doped materials, the photoluminescence and decay studies of "donor" ion are performed. Such approach allows to estimate a theoretical quantum yield under assumption of an ideal cooperative energy transfer. However, the values of quantum yield obtained in such a way are unattainable for real materials.

To get better understanding of the energy transfer process in the oxide materials co-doped with Bi^{3+} and Yb^{3+} , direct measurements of external quantum yield were performed along with studies of photoluminescence, photoluminescence excitation, and photoluminescence decay kinetics. In particular, Gd_2O_3 :Bi,Yb and $Y_3Al_5O_{12}$:Bi,Yb phosphors have been studied. Obtained results show that the energy transfer process in Gd_2O_3 :Bi,Yb is non-cooperative, i.e. an ordinary down-shifting mechanism occurs in this material. At the same time, for YAG:Bi,Yb, our results testify the cooperative energy transfer process from one Bi^{3+} ion to two Yb³⁺ ions.

[1] T. Trupke, M.A. Green, P. Wurfel, J. Appl. Phys. 92, p.1668-1674 (2002).

^[2] Y. Zhydachevskii, L. Lipińska, M. Baran, M. Berkowski, A. Suchocki, A. Reszka, *Mater. Chem. Phys.* 143, p.622–628 (2014).

Acknowledgments: The work was supported by the Polish National Science Center (project 2015/17/B/ST5/01658) and by the EU within the European Regional Development Fund through the Innovative Economy grant (POIG.01.01.02-00-108/09).

The Effect of Ytterbium Content on Properties of ZrO₂:Pr, Yb Nanoparticles Prepared by Microwave Hydrothermal Method

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In recent years, the interest in the nanoparticles based on the metal oxides and rare-earth doping is conected with its widespread practical application possibilities. Especially, they are very interesting objects in various potential applications in biology and medicine. A lot of attention is focused on zirconium oxide ZrO_2 doped with rare-earths (RE) due to its excellent mechanical, electrical and optical properties. Pure zirconia is wide band-gap semiconductor with low phonon frequencies. It makes this compound an adequate host for rare-earths. Substitution of zirconium ions by low-valent and rare earth cations causes oxygen vacancies formation and may stabilize other phases. Furthermore, zirconia was proven to be non-toxic and biocompatibile material, which may be used as a base for luminescence markers, biosensors and drug delivery systems. Among Rare Earths the Yb³⁺ ions have a very simple energy-level diagram containing only two states: ${}^2F_{7/2}$ and ${}^2F_{5/2}$, which are conected with spin-orbit coupling. In our work, Yb³⁺ ions had not only the function of a stabilizer, but also are sensitizers to activate Pr³⁺ ions for up-conversion luminescence.

In the current research, ZrO_2 nanopowders doped with 0.5 mol% of Pr nad x mol % of Yb (x = 0.5, 1, 2, 4, 8, 12, 16, 20 mol %) were prepared by microwave hydrothermal synthesis. This relatively simple and easy controlled method is one of the new techniques for producing nanopowders with a narrow size distribution and controlled morphology [1]. Hydrothermal method allows crystallization of oxides in aqueous environment and offers a lot of advantages. Mainly, materials obtained by this technique exhibit high-quality and purity.

The effect of ytterbium content on the morphologies, crystal structures and optical properties of ZrO₂: Pr, Yb nanoparticles were characterized by Scanning Electron Microscopy (SEM), X-Ray diffraction (XRD), catodo-(CL) and photoluminescence (PL) spectroscopy.

Our results confirmed change of structural and spectroscopic properties with increasing ytterbium content. By applying X-ray diffraction, the dopant effect on the zirconia phase stability was found. A change of the crystalline phase from monoclinic to tetragonal/cubic was observed with increasing Yb^{3+} concentration, especially for annealed samples. From PL and CL investigations it was found that the luminescence of Pr^{3+} ions was less intense for samples with a higher content of Yb^{3+} ions. Infrared to visible up-conversion luminescence was obtained at 975 nm excitation.

[1] Byrappa K., Masahiro Yoshimura: Handbook of hydrothermal technology. A technology for crystal growth and materials processing. Wiliam Andrew Publishing, LLC, New York, USA (2001).

Acknowledgments: This work was supported by National Science Centre, grant numbers: 2012/05/E/NZ4/02994 and 2012/06/A/ST7/00398.

Optical Studies of BaWO4:Ce,Na

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Investigated BaWO₄ crystals were specifically oriented and grown using Czochralski method. After doping with trivalent cerium ions those materials exhibit relatively new properties in matters of stimulated Raman scattering – they can serve simultaneously as effective Raman shifter and efficient scintillator. Synthesized single crystals also possess scheelite-like structure (SG I4₁/a) in which lack of charge, after Ba²⁺/Ce³⁺ substitution, is compensated by structural defects or alkaline ions such as Na⁺.

Experimental results show that crystals have prominent absorption from Ce^{3+} ions peaked at 320 nm - this band is certainly associated with lowest 4f-5d energy transfer. Smaller signal at 285nm is purely assigned to tungstate exciton from inside the host. We try to establish what is the sole mechanism of elongated green luminescence during pressure elevation since it's not clearly related to Ce^{3+} and even though this material has the biggest band gap from all known family of tungstates, it shows no prominent emission in ambient conditions. We assume that changes in PL with compression are related to closing of large BaWO₄ band gap and photoionization of W⁶⁺ 5d states with the hosts conduction band.

Raman spectra support these results showing second order phase transition occurring in between 7 (metastable Fergusonite – SG I2/a) and 9 GPa (monoclinic BaWO4-II – SG P2₁/n) after which green emission starts and further intensifies. Prominent hysteresis during decompression is also worth noticing since it has its impact on elongated PL effect.

In infrared spectra several, sharp absorption lines could be observed with their origin associated with multiple, different Ce multisites and their internal 4f-4f transitions. These signals are also strongly coupled with nearby lattice vibrations and they undergo prominent sharpening with decreasing temperature.

^[1] P. Černý et. al., IEEE J. Quantum Electron., 38, 1471 (2002),

^[2] D. Ran et.al., Cryst. Res. Technol., 41, 1189 (2006),

^[3] K.V. Dabre et. al., J. Lumin., 149, 348 (2014)

Eu³⁺ Luminescent Centers in RE=Y, Gd, Tb Aluminum Perovskites under High Pressure

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In current work, the YAIO₃ GdAIO₃ and TbAIO₃ perovskites doped with trivalent europium were investigated. These materials in the form of the single crystalline film (SCF) are perspective as scintillating screens for microimaging applications. SCF samples were prepared by liquid phase epitaxy method from the melt solution based on the PbO-B₂O₃ flux onto YAP substrates. The structural quality of films was studied using X-ray diffraction.

In other recent investigations [1] it was shown, that in RAIO₃ perovskite compounds with different R=Y, Lu, Gd cations, Eu³⁺ tends to occupy various sites with various local symmetry. In order to better understand this phenomenon, high-pressure luminescence measurements were performed. So called asymmetry ratio for ${}^{5}D_{0} \rightarrow {}^{7}F_{2}$ and ${}^{5}D_{0} \rightarrow {}^{7}F_{1}$ transitions was calculated as $K = I({}^{5}D_{0} \rightarrow {}^{7}F_{2})/I({}^{5}D_{0} \rightarrow {}^{7}F_{1})$ for pressures up to 16 GPa. It was revealed, that for GdAP:Eu and TbAP:Eu perovskites, the K value have the tendency to change with increase of pressure but for YAP:Eu we not observed the changes of K values with pressure.

We have found that K-value at ambient pressure is in good agreement with [1]. In [1], luminescence originating from transitions ${}^{5}D_{1} \rightarrow {}^{7}F_{j}$ was measured at room temperature. In our work luminescence associated with ${}^{5}D_{2} \rightarrow {}^{7}F_{j}$ transitions are also clearly observed. For GdAP:Eu and TbAP:Eu all lines in luminescence spectra shift to the lower energies with increase of pressure. Only one ${}^{5}D_{0} \rightarrow {}^{7}F_{0}$ line was detected in GdAP:Eu and TbAP:Eu SCFs. For this reason, we have concluded that Eu occupies only one site in these perovskites [2].

In the case of YAP:Eu, there are at least three lines, related to ${}^{5}D_{0}\rightarrow{}^{7}F_{0}$ transitions. That means that Eu occupies multiple sites in this material [2]. Another difference is observed in luminescent properties of YAP:Eu, connected with shift to the higher energies of the lines originating from ${}^{5}D_{0}\rightarrow{}^{7}F_{2}$ and ${}^{5}D_{1}\rightarrow{}^{7}F_{2}$ transitions and shift to the lower energies of the lines related to ${}^{5}D_{0}\rightarrow{}^{7}F_{1}$ and ${}^{5}D_{1}\rightarrow{}^{7}F_{1}$ transitions, with increase of applied pressure. The nature of observed behavior is assigned to changes of local symmetry of different Eu³⁺ sites under pressure [3].

- [2] Peter A. Tanner, Chem. Soc. Rev., 42 (2013) 5090.
- [3] A. Kaminska, R. Buczko, W. Paszkowicz, H. Przybylińska, E. Werner-Malento, A. Suchocki, M. Brik, A.
- Durygin, V. Drozd, S. Saxena, Phys. Rev. B. 84, 075483 (2011)

^[1] V. Gorbenko et. al., CrystEngComm, 20 (2018) 937-945.

Hole Trap Process and IVCT Interfered High Sensitive Optical Thermometry in Pr³⁺ Doped Na₂La₂Ti₃O₁₀ Micro-crystals with Layered Perovskite Structure

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In this work, we demonstrated a high-sensitivity optical thermometric material based on the diverse thermal quenching behaviors in the Ruddlesden-Popper type perovskite Na₂La_{1.995}Pr_{0.005}Ti₃O₁₀ miro-crystals, which provide a perspective approach to design self-referencing optical temperature sensing materials with superior temperature sensitivity. The fluorescence intensities ratio (FIR) of Pr³⁺ ${}^{3}P_{0}$ and ${}^{1}D_{2}$ multiplets, host-sensitized and IVCT state interfered, reveals outstanding temperature sensing performance with the maximum relative sensitivity as high as 2.43% K⁻¹ in high-temperature range from 296 to 533 K. Interestingly, it is found that ${}^{3}P_{1}$ and ${}^{3}P_{0}$ levels of Pr³⁺ can be explored as thermally coupled energy levels (TCEL) for thermal sensing with relatively high sensitivity in the low-temperature range from 150 to 275 K. Furthermore, the spectral characteristic of low-temperature luminescence exhibits the efficient energy transfer from host to activator Pr³⁺ ions under band-gap excitation. The results suggested that Pr³⁺ ions work as hole trap and recombination sites for efficient energy transfer from host to Pr³⁺ ions under band-gap excitation energy transfer from host to Pr³⁺ ions. In addition, thermoluminescence, decay kinetics and high-pressure of luminescence were also performed to confirm our interpretation of experimental results and the model proposed for the system. This work on the luminescence properties of layered perovskite compound can be expected to lead to the development of new photofunctional materials.

Mr. Landau and Mr. Zener in Silicon Valley

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Recently quantum two-state systems, known as the qubit can be among others realized in so called gated quantum dots, where the electron is singled out by a potential well created by sclassical circuit [1]. Due to limited scalability of such architecture, the protocols of sending quantum information between arrays of such devices are currently investigated [2].

In my talk I would like to give a quick detour, and advertise how a single electron can be shuffled between two, gated quantum dots in Silicon, and show how such problem becomes equivalent to celebrated Landau-Zener transition [3]. Apart from introducing a toy-model, I would gradually investigate how environmental properties like valley-splitting, noise or roughness of the heterostructure interface, affect the transfer success.

- [1] E. Kawakami et al., Electrical control of a long-lived spin qubit in a Si/SiGe quantum dot, Nature Nanotechnology **9**, 666-670 (2014).
- [2] Si QuBus project: https://www.quantera.eu/co-funded-call/funded-projects/58-si-qubus.
- [3] X. Zhao, X. Hu, Coherent electron transport in silicon quantum dots, arXiv: 1803.00749 (2018).

NV center spin qubit as a sensor of nanoscale environment

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Ouantum properties of a qubit have a finite lifetime because of the interaction with an environment. On the other hand, due to high sensitivity on fluctuations inside the environment, qubit can become an antenna. Experimental work in this direction, such as probing the organic molecules [1, 2] are realized using a nitrogen-vacancy (NV) center - a deep defect in diamond, which bonds a free electron pair (coming from nitrogen) in a complex with vacancy. Such defect can be prepared in a pure quantum state, using visible light in room temperature. Then its spin state is controlled using microwaves, NV center, prepared in superposition state, decoheres within microseconds, without any additional control. Application of Dynamical Decoupling (DD) techniques, used widely in NMR, not only help in elongating the qubit lifetime, but also can become a filter of a given frequency. DD corresponds to a sequence of qubit rotations, applied periodically with free qubit evolution time τ , which can be directly translated to a characteristic frequency $\omega_f = \pi/r$. Now, when we tune this frequency to Larmor precession of some nuclei, present in the environment, we cause the qubit to be specifically sensitive to interactions of those nuclei. Also, some modifications of DD method for quantum sensing were proposed [3]. First one measures a correlation between two above described sensing periods, separated by some time, when a qubit is rotated on such a direction that it becomes less sensitive on external fluctuations. The measured signal contains information about the nuclei precession frequency or even qubit-nucleus interaction strength. Recently, there was another proposal for nanoscale environment sensing, called QDyne [4]. It uses dynamical decoupling, but also subsequently a measurement of the qubit state and reinitialization of its superposition. Then, the whole sensing-measurementinitialization sequence is repeated. If the signal is highly coherent, continuous repetition of measurement, finally produces a spectrum of classical environment, with very high accuracy depending only on the total time of such experiment, which can be arbitrarily long. Those new techniques seem to be promising for increasing sensitivity and spectral resolution. However, introducing additional operations on qubit, especially a series of projective measurements, opens a new set of questions for exploitation of those for sensing a quantum mechanically described environment, consisting of nuclear spins.

- [1] T. Staudacher, et al., Science 339, 561 (2013),
- [2] I. Lovchinsky, et al., Science 351, 836-841 (2016),
- [3] A. Laraoui, et al., Nat. Comm. 4, 1651 (2013),
- [4] S. Schmitt, et al., Science 356, 832 (2017).

Coarse-grained model of intrinsically disordered proteins

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Intrinsically disordered proteins (IDPs) play an important role in cell-cycle regulation, signaling, transcription and translation [1]. They don't have one clearly defined structure and can adopt different conformations, depending on their environment. Therefore, a model of an IDP cannot be fully structure-based [1]. However, it can rely on statistical properties of a conformational ensemble of IDPs, obtained from all-atom simulations or experiment. I will present such a model, where one pseudo-atom represents one amino acid, local interactions (between pseudo-atoms adjacent in the protein chain) are based on random protein coil library [2], and nonlocal interactions (between pseudo-atoms not close to others in the chain) are modeled either by Lenard-Jones potential, similar to that used in the structure-based model [3] or by screened electrostatic potential for charged amino acids. Our model was parametrized using a mix of experimental and all-atom simulation data for homopolymers, which are IDPs. Among them polyglutamine was given special attention, because polyglutamine tracts in some proteins are responsible for various neurodegenerative diseases and are known to aggregate into amyloids [4]. The model was also used to model gluten, a set of IDPs from wheat grains, responsible for dough elasticity, rich in glutamine [5].



Fig. 1: One of modeled polyglutamine structures

- [1] J. N. Johnson, E. Ahrendt and J. E. Braun, *Biochem. Cell Biol.* 88(2), 157–165 (2010).
- [2] A. Ghavami, E. Giessen and P. R. Onck, J. Chem. Theory Comput. 9(1), 432-440 (2013).
- [3] J. I. Sułkowska and M. Cieplak, *Biophys. J.*, **95**, 317491 (2008).
- [4] À. Gómez-Sicilia, M. Sikora, M. Cieplak and M. Carrión-Vázquez, PLoS Comput. Biol. 11(10), 1-4 (2015).
- [5] H. Wieser, Food Microbiol. 24(2), 115–119 (2007).

Modified upconverting NaYF₄ nanoparticles for photodynamic therapy

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Over the last few years, the photodynamic therapy (PDT) using upconversion nanoparticles (UCNPs) has generated a substantial surge of interest. In particular, it has been demonstrated that UCNPs based on lanthanide-doped NaYF₄ with covalently attached molecules of selected photosensitizers (UCNPs-PS) are capable of generating reactive oxygen species (ROS) upon irradiation with near infrared (NIR) laser light. Specifically, it has been shown that the formation of ROS occurs via the Förster Resonance Energy Transfer (FRET) from UCNPs to the attached PS molecules. The elevated concentrations of ROS in the targeted cells might cause cellular damage, thus opening an avenue for NIR-light induced in vivo PDT of diseased tissues, including treatment of cancers.

The goal of this study was to develop the multifunctional UCNPs-PS based on NaYF₄:20%Yb,2%Er. Our work encompassed the synthesis of UCNPs and functionalization of their surface towards obtaining UCNPs-PS nanoconstructs. It was then followed by evaluation of the photo-physical characteristics of the thus obtained UCNPs-PS nanoconstructs and testing of their biological impact –from the perspective of their further medical applications.

Multifunctional, NIR-light-active photoluminescent and ROS-generating UCNPs-PS nanoconstructs were synthesised and characterized. Firstly, UCNPs based on NaYF₄:20%Yb,2%Er were encapsulated in silica (SiO₂). Then, the SiO₂ surface of UCNPs was functionalized with amine groups. Lastly, the molecules of a well-established ROS-generating dye, Rose Bengal (RB), were attached, thus leading to NaYF₄:20%Yb,2%Er@SiO₂-RB nanoconstructs. The upconversion luminescence (UCL) decay times of the the thus obtained UCNPs-PS nanoconstructs were measured. The energy transfer (FRET) from UCNPs to RB molecules was demonstrated. Finally, the biological tests of UCNPs-PS nanoconstructs were performed. The NIR-light induced ROS generation was confirmed by spectro-photometric methods.

The obtained results point to prospective promising applications of the herein synthesized $NaYF_4:20\%Yb,2\%Er@SiO_2-RB$ nanoconstructs in biomedicine. We demonstrated that these UCNPs-PS nanoconstructs were capable of producing ROS upon NIR light irradiation. Further surface modifications with specific antibodies will improve the target-specificity of such UCNPs-PS nanoconstructs, thus leading to molecular-targeted anti-cancer therapy.

[1] Guo, Y.; Rogelj, S; Zhang, P., Nanotechnology 21 (2010) 065102,

[2] Liu, K.; Liu. X.; Zeng, Q.; Zhang, Y.; Tu, L.; Liu, T.; Kong, X.; Wang, Y.; Cao, F.; Lambrechts SA; Aalders MC; Zhang, H.; *ACS Nano.* 2012 May 22;6(5):4054-62.

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Heat-induced degradation of fibrils: Exponential and sigmoidal kinetics

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The degradation of amyloid beta fibrils by thermal fluctuations is studied using the analytical theory and molecular simulations. The logistic like equation, where the impact of fibril size is taken into account, has been developed to mimic different scenarios. In the case when detached monomers are captured for small enough protofibrils, in agreement with experiment, the time dependence of the number of monomers that belong to the dominant cluster is described by the single exponential function. In the opposite case we obtained a sigmoidal behavior. In the case of recycling for both large and small protofibrils the degradation of the dominant cluster follows the logistic behavior. We have shown that the time dependence of fibril contacts is described by a bi-exponential function, in the line with experiments on ThT fluorescence.

Non-obvious Synthesis of Amido-Coumarins and Their Photophysical Properties

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Aromatic oligoamides are intensively explored since they form an amazing variety of discrete architectures such as helixes, tapes and molecular electrets [1,2,3]. The main driving forces responsible for the stacking of such systems are dipol-dipol and π - π interactions. The very special case of such interactions has been recently encountered by us [4]. The CoumDimer comprised of two coumarin units linked by tertiary amide bridge was the first example in which two polarized coumarin units are linked together by amide bridge in head-to-tail orientation. Using single, sterically hindered coumarins as a building block, we wanted to obtain a structure with linearly arranged molecular units. But it turned out that privileged conformation is a structure in which the coumarin units form a wedge. This situation prompted us to perform in-depth studies of photophysical properties of the family of dimeric structures comprised of two coumarin moieties linked in head-to-tail orientation.

The key goal was the modification of spatial arrangement of both coumarin units via introduction of a hydrogen bond. We designed and synthesized three new coumarin dimers (Fig. 1). Herein we would like to present non-trivial synthesis of these molecules as well as its intriguing photophysical properties, which are supported by theoretical calculations.



Fig. 1: Coumarin dimers.

[1] D. W. Zhang, X. Zhao, J. L. Hou and Z. T. Li, Chem. Rev. 112, 5271-5316, (2012),

[2] P. N. Wyrembak and A. D. Hamilton, J. Am. Chem. Soc. 131, 4566-4567, (2009),

[3] B. Xia, D. Bao, S. Upadhyayula, G. Jones II and V. I. Vullev, J. Org. Chem. 78, 1994-2004, (2013),

[4] Ł. Kielesiński, O. Morawski, Ł. Dobrzycki, A. L. Sobolewski and D. T. Gryko, *Chem. Eur. J.* 23, 9174-9184, (2017).

In-Situ TEM Annealing Experiment of Core-Shell Semiconductor Nanowires

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For over two decades, there has been intensive search for new spintronic materials combining semiconducting and ferromagnetic properties at room temperature. The studies on dilute ferromagnetic semiconductors (DFS), have shown so far, that (Ga,Mn)As grown in the form of thin epitaxial layers reaches remarkably high Curie temperature ~ up to 190K (Tc) as for DSF material, but still too low for application. However, its potential can be used after a thermal treatment resulting in hybrid material – the semiconducting matrix (Ga,Mn)As with intermetallic MnAs (ferromagnetic<40°C) nanoprecipitates.

In our previous studies [1], we showed that it is possible to obtain (Ga,Mn)As in hexagonal wurtzite (WZ) structure as a form of cylindrical epitaxial shell around WZ (Ga,In)As core of the nanowire (NW) in molecular beam epitaxy process. Ex-situ post-annealing of such NWs revealed that above 450°C in (Ga,Mn)As shells, hexagonal MnAs nanoprecipitates arise coherently in the WZ matrix. To determine how the formation of MnAs precipitates occurs in the WZ core-shell (Ga,In)As/(Ga,Al)As/(Ga,Mn)As/LT-GaAs, the in-situ experiment is performed in transmission electron microscope (TEM) using heating chips and double tilt holder. Our study shows that structural changes in WZ NWs start from Mn atoms segregation in WZ lattice at temperatures around 300°C (Fig.1ab) and are followed by phase transition to hexagonal MnAs precipitates semi-coherent with WZ-GaAs matrix over 400°C (Fig.1cdef). At higher temperatures, the precipitates have the same orientation as the matrix and we observe their growth with visible Moiré pattern and additional voids creation (Fig.1gh). The decomposition of NWs occurs above 550°C (Fig.1ijkl).



Fig. 1: Scanning Transmission Electron Microscopy (STEM) images of the typical WZ NW placed on the heating chip and its structural changes while in-situ annealing measurements in: a,b) 350°C c,d) 400°C e,f) 450 °C g,h) 500°C i,j) 550°C k) over 600°C l) HRTEM image of one MnAs nanoprecipitate.

[1] J. Sadowski, Nanoscale 9, 2129 (2017)

Electron Holography Methods for Investigation of Magnetic Nano-objects

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When plane electron wave passes through a sample it is affected by electric and magnetic fields. It can be shown that the effect of magnetic field can be described as follows: $\Psi(\vec{r}, t) = \Psi(\vec{r}, t) e^{ig(\vec{r})}$, where $\Psi(\vec{r}, t)$ is a wave function in the absence of magnetic field and $g(\vec{r}) = \frac{e}{\hbar} \int \vec{A}(\vec{r}) d\vec{r}$ is a phase shift corresponding to magnetic field's presence. Definition of $g(\vec{r})$ involves a vector potential \vec{A} which corresponds to the induction of magnetic field $\vec{B} = \nabla \times \vec{A}$.

Electron holography allows to determine phase of wave function. Therefore it makes possible to separate phase shifts introduced to the electron wave by electric and magnetic fields. In practice it can be accomplished if two electron holograms are recorded, each one for a different interaction with magnetic field. Most common method is to record one hologram for an upside- and another one for a downside orientation of a sample. In that case electric field deflects electrons in the same direction no matter what the sample orientation is. On the other hand, the inversion of sample causes the Lorentz force vector to change the direction to opposite. Hence, the sum of phases refined from two holograms will contain only the "electric" phase part, while their subtraction will correspond to the phase shift caused by magnetic field.

Due to the fact that sample is turned upside down manually, two holograms showing the same area may be misaligned and differently scaled. Often it is necessary to apply image operations such as shift, rotation and rescaling, because small misalignments between holograms may produce significant artifacts in restored phases. In order to unify and speed up the process of hologram analysis a dedicated software was developed, which semi-automatically aligns holograms and uses them to refine magnetic phase shift. Internal electric and magnetic fields were determined for $Nd_7Fe_{75}B_{14}Nb_4$ alloy sample (Fig. 1). Basic theory behind electron holography as well as software for reconstruction of recorded holograms will be presented.



Fig. 1: Electric (a) and magnetic (b) fields refined from two holograms acquired for $Nd_7Fe_{75}B_{14}Nb_4$ alloy sample.

High Resolution X-ray Diffraction Characterization of Novel Ca₃RE₂(BO₃)₄ (RE = Y, Gd) Single Crystals

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In recent years, rare earth containing borates are studied as materials applicable for optoelectronic devices [1]. In particular Pan et al. reported that Nd-doped disordered $Ca_3Gd_2(BO_3)_4$ crystal is a promising disordered laser material [2]. The crystallographic quality (point defects, dislocations, small voids or inclusions, micromosaics, block structure etc.) strongly influences the physical properties of the solid. The available information on the crystal quality of rare earth containing borates is scarce. This justifies the need of detailed studies of the nature of possible defects.

The present work is devoted to high-resolution X-ray diffraction characterization of Czochralskigrown $Ca_3RE_2(BO_3)_4$ (RE = Y, Gd) single crystals, using the $CuK_{\alpha 1}$ radiation (1.5406 Å). The samples are known for the lack of gas bubbles inclusions and impurity phases [3]. They are evaluated in terms of a structural perfection degree. The defect structure is recognized and compared with the literature data concerning similar single crystals of related composition and/or structure.

The preliminary information about chemical homogeneousness of the samples was obtained from the 2θ - ω scans. The width (FWHM) of rocking curves was between 40 t o70 arcsec, proving a high level of a structural perfection of the crystals. Reciprocal space mapping enabled the lattice defects identification – they are micromosaics and block structure; the spatial variation of lattice parameter gave an indirect information about the chemical composition distribution. The study shows that the Ca₃RE₂(BO₃)₄ (RE = Y, Gd) crystals can be Czochralski-grown with quality suitable for considering them as components of optoelectronic devices.

[1] T. N. Khamaganova, Russ. Chem. Bull. 66, 187 (2017),

[2] Z. B. Pan, H. J. Zhang, H. H. Yu, M. Xu, Y. Y. Zhang, S. Q. Sun, J. Y.Wang, Q. Wang, Z. Y. Wei, and Z. G. Zhang, *Appl. Phys.* **106**, 197 (2012),

^[3] L. V. Gudzenko, M. B. Kosmyna, A. N. Shekhovtsov, W. Paszkowicz, A. Sulich, J. Z. Domagała, P. A. Popov, and S. A. Skrobov, *Crystals* **7**, 88 (2017).

Strain Relaxation of InGaN Epitaxial Layers

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III-nitrides such as AlN, GaN and InN have gained importance in the production of optoelectronic devices. Alloying of these compounds should enable a change in the color of the emission wave in the range from ultraviolet to red. However, the growth of high indium content InGaN layers remains one of the challenges in III-nitrides development. There are theoretical studies showing that introduction of higher amounts of In in the InGaN layers requires substrates with higher lattice constant than commonly used GaN substrates.[1] The idea of using relaxed InGaN layers deposited on GaN templates as pseudo-substrates for the growth of InGaN-based structures has recently emerged.[2]

The basic mechanism for strain relaxation is the generation of misfit dislocations at the layer/substrate interface. Due to the impact of dislocations on material properties, understanding of the dislocation formation mechanism is crucial for the production of the devices. Till now only a preliminary study on the strain relaxation mechanisms has been performed in case of III-nitrides group of materials. Moreover there are inconsistencies in the existing literature concerning the kind of the dislocations which relax these structures.

In this work we study relaxation mechanism of InGaN layers grown on (0001)-oriented GaN substrates using different techniques of transmission electron microscopy (TEM), high resolution x-ray diffractometry (XRD) employing reciprocal space mapping as well as cathodoluminescence imaging in scanning electron microscope (SEM).

We discuss peculiarities of plastic relaxation of InGaN epilayers and their consequences for pseudo-substrate application. We unambiguously determine the misfit dislocation type and show that layers exhibit anisotropic state of strain relaxation. We reveal that post-growth annealing may be a useful tool for an increase of the state of strain relaxation, however, we found the limit for achievable degree of relaxation.

[1] A. I. Duff et al., *Physical Review B* **89**, 085307 (2014),

[2] K. Hestroffer et al., Semiconductor Science and Technology 30, 105015 (2015).

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Point defects in GaN:Si grown by MOVPE and their influence on decomposition of InGaN QWs

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In the MOVPE, the InGaN quantum wells which are the active part of Light Emitting Diodes (LEDs) and also Laser Diodes (LDs) must be grown at temperatures of 700-750°C, whereas good p-type layers doped with Mg (Mg is the only acceptor in nitrides) can be obtained at much higher temperatures in the range of above 900°C. Unfortunately, when p-type is grown at high temperature, the InGaN quantum wells get decomposed. Fig. 1 Left: shows examples of InGaN MQW



decomposition after p-type growth.

Fig. 1: Left: InGaN quantum wells decomposed after p-type deposition at high temperatures. Left: Transmission Electron Microscopy (TEM) (nanometer scale). Right: Photoluminescence of three samples grown at different temperatures and pressure in nitrogen atmosphere.

The most interesting feature is that the decomposition of InGaN MQWs starts usually from the first quantum well. Careful PL/EL (photo-/electroluminescence) and XRD and also TEM examinations of the first stages of the InGaN QW decomposition enabled us to propose a microscopic model of the InGaN QW decomposition. The model consists of the following steps: (1) The diffusion driven homogenization of the InGaN alloy, (2) The formation of voids, (3) Decomposition of the InGaN surrounding the voids, (4) Recrystallization of the etched areas. According to this model, decomposition phenomenon is caused by strain-driven, built-in electric-field-driven diffusion of In/Ga/N vacancies. Due to this examination of point defects and their diffusion in Si doped GaN is the crucial point of this problem, because it is the layer on which the InGaN QWs are grown. In this work we investigated low doped n-GaN layers prepared by MOCVD on sapphire template at different growth conditions: temperature, pressure, in hydrogen or nitrigen atmosphere. PL spectra measured in wide range, Fig.1 Right, show us the signal of yellow PL growing due to increasing amount of V_{Ga}. Due to the low Si content, these layers will be also measured using the DLTS technique to confirm presence of V_{Ga} and identify other defects in MOVPE growth. Resulted net doping donor concentration is well controlled of level of 10¹⁷ cm⁻³. In future work will be grown samples with higher Si doping which allow examine how point defects depending (their amount and kind) on the amount of intentional doping.

Technological approach to vertical transport structures based on GaN epilayers

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Theoretical prediction suggest large spin filtering capabilities of spin filters and resonant tunneling diodes involving insulating ferromagnetic barriers. The tunneling spin-filter effect in a metal/ferromagnetic insulator/metal tunnel junction take place when electrons with randomly oriented spins tunnel from the Fermi level of the nonmagnetic metal through the spin-dependent barrier. The spin-split conduction band of ferromagnetic part creates a lower barrier height for spin-up electrons and higher barrier for spin-down electrons, giving rise to a highly spin-polarized current (Fig. 1).

In our approach to spin filtering concept we want to employ devices made of structures containing GaN:Si/(Ga,Mn)N/GaN:Si, where (Ga,Mn)N is a thin ferromagnetic layer and the whole stack is epitaxially grown on sapphire substrates. On the other hand the lattice mismatch between sapphire and GaN results in a sizable number of vertically oriented misfit-related threading dislocation which are highly conductive so they are shortening the researched nonlinear characteristics. One of the way to reduce this detrimental effect is to shrink the active area of the device to a micrometer-size range. Our current approach is schematically drawn in Fig. 2. We employ a mask made of a dielectric oxide (Al₂O₃ or HfO₂) deposited on the free surface of the structure by the atomic layer deposition method. In this ~50 nm thick insulating layer windows of 5 to 10 micrometers are defined by the lift-off method. These windows are now covered by a larger in diameter gold contacts which make only a local electrical contact with the GaN-based structure, yet they constitute a sufficiently large conductive platform to which electrical wires can be conveniently bonded. This technological effort is the first step towards elaboration of fully operational submicrometer devices.



Fig 1: Scheme of the spin filter, tunneling through a spin dependent barrier.

Fig 2: Scheme of the contacting of micrometer size vertical transport devices using an insulating oxide mask (gray-sample, blue-aluminum oxide, yellow-gold contact pads).