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Abstracts

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Structural and magnetic properties of ferromagnetic Co ultra-thin films - ^{59}Co NMR studies

Przemysław Nawrocki

Supervisor: prof. Marek Wójcik

The results of ^{59}Co Nuclear Magnetic Resonance measurements on two systems based on Co ultra-thin films, which can have extensive spintronic applications, are presented. The first series of samples were hcp Co(0001) films epitaxially grown on an Au(111) buffer and capped with an Au layer with Co layer thickness d varying from 1,5 nm to 10 nm. The aim of this study was to examine structural changes of the Co layer as a function of thickness and to investigate interface effects due to strain induced by the lattice mismatch between Au and Co, which may influence the magnetic anisotropy. It was found that Co layers with $d<3$ nm make atomically sharp interface to Au(111) substrate in major part of the contact area. Co atoms located inside a bulk of the layer reveal a higher resonance frequency than reported for a bulk sample (226 MHz) which suggests that the Co layer is under a tensile strain. For thicker layers with $d\geq3$ nm a transition to a relaxed hexagonal structure with an increased amount of grain boundaries takes place in the entire volume of the Co film. The strain at the interface to Au substrate is relieved by the appearance of additional dislocations and incorporation of Au atoms into the first atomic plane of Co film.

The second series of samples were oxygen implanted polycrystalline 30 nm thick Co films. Ion implantation is a new and very efficient method of inducing exchange bias (EB) in the whole volume of Co thin layers. The films were grown on an Au buffer and capped with an Au layer. The samples were subsequently implanted with O ions, with energy of 40 keV, with increasing fluences ranging from 3×10^{16} to 35×10^{16} ions/cm^2 with the aim to produce Co/CoO interfaces spread throughout whole volume of the samples and therefore, to create an EB system. While the as-deposited sample consists of a mixture of fcc and hcp-Co phases and stacking faults (revealed by the spectrum intensity in the range 217–220 MHz), oxygen implanted samples exhibit significantly different structural features. Although there is no allotropic fcc → hcp phase transformation, the metallic Co undergoes a significant loss of crystalline order which increases with implantation fluence (revealed by the progressive shift of the spectrum intensity to frequencies below 200 MHz). For high fluence implantation, presence of CoO can be envisaged from appearance of a new broad ^{59}Co NMR line recorded around 450 MHz. Finally, the ^{59}Co NMR restoring fields of the different samples indicates a significant increase of magnetic stiffness at 4.2 K with growing fluence, which mostly is caused by the EB effect introduced by the presence of antiferromagnetic CoO since this increase of the restoring field is absent at the temperatures above Neel temperature of CoO (e.g. RT).

Magnetic properties of Mn_5Ge_3 modified by carbon

Roger Kalvig

Supervisor: prof. Ewa Jędryka

Hexagonal Mn_5Ge_3 compound, with Mn in two nonequivalent positions: 4d (Mn_1) and 6g (Mn_2), is a prospective spintronic material due to high spin polarization and high Curie temperature (up to 450 K in case of samples doped with carbon). To investigate the magnetic properties of this system, an extensive ^{55}Mn NMR study was carried out on a series of epitaxial films of $Mn_5Ge_3C_x$ for $0<x<0.85$. The NMR spectrum recorded from the pristine Mn_5Ge_3 thin film reveals NMR lines at 210 MHz and 430 MHz, readily attributed to Mn_1 and Mn_2 sites, respectively. Upon the inclusion of carbon, Mn_2 sites are first to be affected, with a new NMR line quickly developing around 355 MHz, indicating a number of Mn_2 atoms with altered magnetic moments. This new value of Mn magnetic moment results from the strong bonding the carbon atoms make with Mn_2 as the nearest neighbors. The effect of carbon is much smaller on Mn_1 sites where it plays the role of a more distant neighbor, and is visible only after reaching a much higher C concentration, close to x=0.5. In order to investigate magnetocrystalline anisotropy we have performed Ferromagnetic Resonance (FMR) experiments. From the angular dependence of resonance field the uniaxial magnetocrystalline anisotropy constants were determined: $3{,}6 \cdot 10^6 \frac{erg}{cm^3}$ for Mn_5Ge_3 and $1{,}24 \cdot 10^6 \frac{erg}{cm^3}$ for $Mn_5Ge_3C_{0.6}$.

Magnetic and Magnetotransport Behavior of $Ge_{1-x-y}Pb_xMn_yTe$ Nanocomposite Crystals

Arkadiusz Podgórni

Supervisor: prof. dr hab. W. Dobrowolski

The structural, magnetic and magnetotransport properties of bulk $Ge_{1-x-y}Pb_xMn_yTe$ samples with variable chemical composition were investigated. The XRD and SEM characterization indicate the presence of two GeTe based phases. Two magnetic phase transitions to spin-glass-like state were found in the studied system with critical temperatures around 80 K and below 20 K, respectively. The magnetometric measurements below T_C showed negative magnetoresistance and anomalous Hall effect. The role of different intrinsic and extrinsic mechanisms responsible for the magnetotransport effect will be discussed.

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Nitrogen doped p-type ZnO films and *p-n* homojunctions

D. Snigurenko

Supervisor: prof. E. Guziewicz

Zinc oxide (ZnO) as a wide band-gap semiconductor shows a huge potential for technological applications since its electric, magnetic and optoelectronic properties can be optimized towards functionalization [1, 2]. Functionalization of ZnO constitutes a crucial step in using this material for electronic, photonic, and sensing applications. ZnO has been considered as a candidate for new sensing nanodevices, which are expected to combine enhanced sensitivity, selectivity, and portability [3].

In this work we present results for polycrystalline ZnO layers grown by Atomic Layer Deposition (ALD) using diethylzinc and deionized water as zinc and oxygen precursors, respectively. As a substrate we used silicon which was uniformly covered with the ZnO film in a double exchange reaction between precursors. For these films we determined correlation between ALD growth parameters, reduced structural quality and electrical properties [4]. ZnO-ALD films with a very low electron concentration (10^{16} cm^{-3}) have been doped with nitrogen in order to achieve the p-type ZnO. Nitrogen was introduced into the ZnO films by using ammonia water instead of deionized water as an oxygen precursor in the ALD process. In this way the concentration of nitrogen in the ZnO films increased from 10^{18} cm^{-3} (when deionized water was used) to 10^{21} cm^{-3}. The ZnO:N films obtained in this way were highly resistive. The RTA (Rapid Thermal Annealing) in nitrogen or oxygen atmosphere leads to p-type conductivity with a hole concentration at the level of 10^{18} cm^{-3}. The ZnO-based homojunction with p-type and n-type ZnO grown in the ALD processes has been obtained. The rectification ratio of 10^5 is among the best parameters reported for ZnO-homojunctions published so far.

[1] C. Lao, Y. Li, C. P. Wong, and Z. L. Wang, Nano Lett. 7 (2007) 1323

[2] W.Z. Xu, Z.Z. Ye, Y.J. Zeng, L.P. Zhu, B.H. Zhao, L. Jiang, J.G. Lu, H.P. He, S.B. Zhang, Appl. Phys. Lett. 88 (2006) 173506

[3] N. H. Moreira, A. L. da Rosa, T. Frauenheim, Appl. Phys. Lett. 94 (2009) 193109

[4] E. Guziewicz et al. Semicond. Sc. Technol. 27 (2012) 074011

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ZnO/Si photovoltaic structures - new ideas, new results

Rafał Pietruszka

Supervisor: prof. Marek Godlewski

In this work we study PV structures based on n-type ZnO grown at low temperature either by atomic layer deposition (ALD) or hydrothermal method (nanorods). In the first approach, we deposited thin films of n-type ZnO on p-type silicon substrates. Such obtained PV structures of the II generation (ZnO:Al/ZnO/Si/Al) show efficiency of about 6%. In the second approach, we grown ZnO nanorods (ZnO_{NR}) on p-type Si. The growth process was initialed by 15 cycles of ALD process forming ZnO nanoseeds on a Si substrate. Then, the so-deposited ZnO nanoseeds nucleate growth of ZnO nanorods in a hydrothermal process. So-obtained ZnO_{NR} were covered with n-type ZnO and ZnO:Al films by ALD process. The best PV efficiency for such IV generation structures (ZnO:Al/ZnO/ZnO_{NR}/Si/Al) was equal to 12.5%.

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Time-resolved spectroscopy of cerium-doped garnets

Piotr Nowakowski

Supervisor: prof. A. Kamińska

We studied the dynamics of deexcitation processes. We measured the luminescence and decay time of luminescence in GGG:Ce at high pressure (to 10 GPa), at helium temperature in the Streak camera.

Spectra:

We observed the photoluminescence of GGG:Ce in the pressure above the 3 GPa. The PL measurements showed the existence of two 4*f* states of Ce^{3+} ions in the material GGG:Ce.

Kinetics:

Almost constant values of short and long luminescence decay component suggests the phenomenon of pressure induced decrease electron-lattice coupling.

Conclusions:

The observation of short component of luminescence decay indicates the contribution of clear *f-d* transitions (at all pressures where the PL was observed). The observation of long component of luminescence decay suggests the coexistence of anomalous luminescence or the presence of other optically active cerium centers (e. g. Ce^{3+} in octahedral positions).

GaN-AlGaN HEMT structures grown by PAMBE.

Andrzej Cabaj

Supervisor: prof. Z. R. Żytkiewicz

In my speech I present the construction of HEMT heterostructure GaN / AlGaN which was grown by Plasma Assisted Molecular Beam Epitaxy method. After that I shown how to find an optimal conditions for growing GaN and AlGaN high quality layers. In addition, I discuss the impact of Al percentage in the structure HEMT transistor on the parameters of the two-dimensional electron gas - present in the above transistor.

To measure Al mole fraction and strain in $Al_xGa_{1-x}N$, I present XRD results of GaN /AlGaN heterostructure. At the end of my speech I shown measured electrical properties of HEMT structures with and without a thin AlN layer. The results show that thin AlN layer at the interface of GaN/AlGaN heterostructure improves carrier concentration and mobility in 2DEG (2Dimension Electron Gas).

HEMT-grade GaN growth on Si (111) by PAMBE

Giorgi Tchutchulashvili

Supervisor: prof. Z. R. Żytkiewicz

Particularities of Group III nitride-based High Electron Mobility Transistors (HEMT) growth on Si (111) will be discussed. Growth conditions specific for Plasma-Assisted Molecular Beam Epitaxy (PAMBE) are the source of characteristic distortions of layer structure during growth regimes advantageous for latteral growth of GaN. Growth mode of AlN seed layer are shown to be crucial to overcome challenges of HEMT-grade GaN growth on silicon (111) by PAMBE.

Magnetic phase diagram and Critical Exponents of Dilute Ferromagnetic Insulator $Ga_{1-x}Mn_xN$.

Sylwia Stefanowicz

Supervisor: prof. Maciej Sawicki

By using highly sensitive millikelvin superconducting quantum interference device magnetometry, the magnitude of the Curie temperature as a function of the Mn concentration *x* is determined for thoroughly characterized $Ga_{1-x}Mn_xN$ [1]. We assign the spin interactions in this insulator to ferromagnetic superexchange and successfully model our findings in the frame of tight binding theory and Monte Carlo simulations. Moreover we extended the magnetic phase diagram for $Ga_{1-x}Mn_xN$ using MBE grown samples with Mn concentration reaching up to 0.1, which also show excellent crystalline properties [2]. The results fall on the same general trend, indicating basically the same origin of the magnetic coupling in both sets of $Ga_{1-x}Mn_xN$ layers.

We also investigate the static critical behavior of MBE grown (Ga,Mn)N layers with $0.04 < x < 0.10$ by analyzing critical exponents [3]. The critical behavior of this dilute magnetic insulator shows strong deviations from the magnetically clean case (x=1), in particular, (i) an apparent breakdown of the Harris criterion, (ii) a nonmonotonic crossover in the values of the susceptibility critical exponent γ_{eff} between the high temperature and critical regimes, and (iii) a smearing of the critical region, which can be explained either by the Griffiths effects or by macroscopic inhomogeneities in the spin distribution with a variance Δx=(0.2±0.1)%. The obtained value of critical exponents $\beta = 0.6$ and $\gamma = 1.7$ are close, but larger than the expected for XY or Heisenberg universality class.

[1] M. Sawicki, T. Devillers, S. Gałeski, C. Simserides, S. Dobkowska, B. Faina, A. Grois, A. Navarro-Quezada, K. N. Trohidou, J. A. Majewski, T. Dietl, and A. Bonanni, Phys. Rev. B **85**, 205204 (2012).

[2] G. Kunert, S. Dobkowska, Tian Li, H. Reuther, C. Kruse, S. Figge, R. Jakiela, A. Bonanni, J. Grenzer, W. Stefanowicz, J. von Borany, M. Sawicki, T. Dietl,and D. Hommel, APL **101**, 022413 (2012).

[3] S. Stefanowicz, G. Kunert, C. Simserides, J. A. Majewski, W. Stefanowicz, C. Kruse, S. Figge, Tian Li, R. Jakieła, K. N. Trohidou, A. Bonanni, D. Hommel, M. Sawicki, and T. Dietl, Phys. Rev. B **88,** 081201(R) (2013).

Zeeman splitting anisotropy in CdMnTe quantum dots embedded in ZnTe nanowires

Małgorzata Szymura

Supervisor: prof. J. Kossut, dr Ł. Kłopotowski

In this report, we study photoluminescence (PL) of single, semimagnetic CdMnTe quantum dots (QDs) embedded into ZnTe nanowires (NWs). We show that the giant Zeeman splitting of the excitonic transitions exhibits a strong anisotropy depending on the direction of the applied magnetic field (B): the splitting in B oriented parallel to the wire axis being few times larger than for perpendicular field. We interpret this as a result of pinning of the heavy hole (hh) spin to the quantization (i.e., growth) axis, which results in a vanishing hh splitting in perpendicular field.

The samples are grown epitaxially by a vapour-liquid-solid method using gold droplets as catalysts. The NW diameters range from 80 nm to 150 nm and the length is up to 1.8 µm. The presence of CdMnTe insertions results in the appearance of a PL in 1.8 eV–2.2 eV energy range. We show that this broad band consists of individual lines coming from single QDs in NWs. An average linewidth is about 7 meV. Monochromatic mapping of the cathodoluminescence correlates with the scanning electron micrograph, which confirms that the observed emission originates from QDs in NWs and not from any other structures. PL measurements are performed at temperature of 2 K in a cryostat equipped with a double-coil magnet producing magnetic fields at arbitrary angle. In order to apply B parallel and perpendicular to the wire axis, we determine the orientation of the wire by measuring PL linear polarization anisotropy.

Analysis of Binding Affinity of Protein-Ligand Complexes

Son Tung Ngo

Supervisor: prof. Mai Suan Li

Binding of ligands (which are Curcumin, Naproxen, Ibuprofen, 342 compounds derived from Vietnamese plants to Aβ peptide + its fibrils and LVEALYL + RGFFYT to insulin) is studied by docking method and all-atom molecular dynamics simulations. The binding mechanism is studied in detail showing that the van der Waals interaction between ligand and receptor dominates over the electrostatic interaction. The binding free energies obtained by the molecular mechanic-Poisson−Boltzmann surface area method indicate that some of them may be good candidates to inhibit the misfolding process of Aβ and insulin. Our results are in good agreement with the experiments.

Proteins with cavities

Mateusz Chwastyk

Supervisor: prof. Marek Cieplak

We provide theoretical comparisons of the physical properties of eighteen proteins with the pathogenesis-related proteins of class 10 (PR-10) fold, which is characterized by a large hydrophobic cavity enclosed between a curved β-sheet and a variable α-helix. Our novel algorithm to calculate the volume of internal cavities within protein structures is used to demonstrate that, although the sizes of the cavities of the investigated PR-10 proteins vary significantly, their other physical properties, such as thermodynamic and mechanical parameters or parameters related to folding, are very close. The largest variations (in the order of 20%) are predicted for the optimal folding times. We show that, on squeezing, the PR-10 proteins behave differently from typical virus capsids.

Chwastyk, M., Jaskolski, M. and Cieplak, M. (2014), Structure-based analysis of thermodynamic and mechanical properties of cavity-containing proteins – case study of plant pathogenesis-related proteins of class 10. FEBS Journal, 281: 416–429. doi: 10.1111/febs.12611

High power nitride laser diodes grown by plasma assisted MBE

Grzegorz Muzioł

Supervisor: prof. Cz. Skierbiszewski

Laser diodes (LDs) based on III-N materials had found many applications in fields such as optical data storage, pico-projectors, printing etc. All of the commercial nitride LDs are grown by Metal Organic Vapour Phase Epitaxy (MOVPE). In the past few years there was a great progress in development of growth mechanism of GaN and InGaN in Plasma-Assisted Molecular Beam Epitaxy (PAMBE) [1] which had led to the demonstration of violet LDs [2]. This has renewed the interest in MBE technology as a possible alternative to MOVPE in this field.

The great advantage of PAMBE is growth of thick high quality InGaN layers. Application of this layers as waveguides in LDs not only simplifies the epitaxial design but also influences LD parameters providing large optical confinement factor and high beam quality. This allowed us to demonstrate LDs grown by PAMBE operating in the range of λ=430-482nm[3,4].

In this paper we will show recent development of true-blue (λ=450nm) LDs by PAMBE. We will show the impact of epitaxial design on LD parameters such as threshold current density, slope efficiency and characteristic temperature. In particular we will study the influence of electron blocking layer (EBL) design on internal losses and thermal stability.

Optimization of the epitaxial design allows us to demonstrate high power LDs by PAMBE. The maximum optical power achieved at room temperature was 0.5 W per facet. This result together with the long lifetime of LDs grown by PAMBE [3] shows the high potential of this epitaxial technique in commercial nitride LDs.

[1] J. Neugebauer et al., Phys. Rev. Lett. 90, 056101 (2003).
[2] C. Skierbiszewski et al., Appl. Phys. Lett. 88, 221108 (2006).
[3] C. Skierbiszewski et al., J. Phys. D: Appl. Phys. 47, 073001 (2014).
[4] H. Turski et al., Appl. Phys. Lett. 104, 023503 (2014).

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Anomalously weak diffusion of oxygen in GaN at temperatures up to 3400 K and pressures up to 9 GPa

Bogdan Sadovyi

Supervisor: prof. Sylwester Porowski

In this work, the bulk diffusion of oxygen in wurtzite-type GaN crystals at temperatures up to 3400 K and pressures up to 9 GPa is studied. For this purpose the GaN crystals grown by hydride vapor phase epitaxy (HVPE) and having strongly nonuniform distribution of oxygen (as revealed by photo-etching and SIMS measurements), the main donor in GaN, are used. Confocal micro-Raman spectroscopy is applied to estimate free electron concentration from the analysis of plasmon-LO-phonon coupled modes (LOPC). Thereby spatial distribution of free electron concentration is studied by lateral scanning along the cleaved surfaces of the investigated GaN crystals. Thus the HVPE GaN crystals studied are shown to contain heavily doped ($n \sim 2.0 \div 4.0 \cdot 10^{19}$ cm^{-3}) and undoped ($n \leq 10^{17}$ cm^{-3}) areas having sharp step-like carrier concentration profiles in micrometer scale. Annealing at high temperatures and high pressures results in only slight diffusion blurring of the carrier profiles at a distance less than 10 □m from the interface. Extremely small values of diffusion coefficient $D \leq 6.3 \cdot 10^{-13}$ m^2/s ($T = 3400$ K and $P = 9$ GPa) estimated from the measured diffusion length are in good agreement with K. Harafuji's molecular dynamic calculations [1], confirming the anomalously small diffusion coefficient in the N-sublattice of GaN.

1. J. Appl. Phys. 96, 2501 (2004).

Thermal properties of layered cobaltites RBaCo$_2$O$_{5.5}$ (and potential application of these materials in fuel cells)

J. Więckowski, A. Szewczyk, M. Gutowska, K. Conder,
E. Pomjakushina, V. P. Gnezdilov, S. L. Gnatchenko.

I presented the part of the results of my doctor thesis *„Właściwości cieplne i magnetyczne wybranych związków kobaltu o strukturze warstwowej”*.
I talked about the results of specific heat studies of a series of RBaCo$_2$O$_{5.5}$ (R = Y, Gd, and Tb) layered cobaltites. These studies were aimed at explaining an influence of different rare-earth ions on thermal properties of these compounds and at studying phase transitions appearing in them.
The specific heat studies were performed over the temperature range from 3 to 395 K, in the magnetic field ranging from 0 to 9 T. Anomalies accompanying different phase transitions were analyzed. Lattice, magnon, and Schottky contributions to the specific heat were separated and described theoretically. The molecular field corresponding to the R–Co exchange interactions was estimated to be ~ 1 T.