Workshop

"Fundamental research – New Materials"

Organized by the EU COST Action OPERA

Madrid, April 19-21, 2023

OPERA
COST Action CA20116

Dear colleagues,

It is our great pleasure to welcome you to the **OPERA Workshop "Fundamental research – New Materials"**, **Madrid-Spain**.

This Workshop covers the scientific tasks of the Action related to the Work Group 1 by taking an interdisciplinary and cross-community approach to key developments in epitaxy, new theoretical and experimental for the maturation of epitaxial materials, and novel functionalities for next-generation devices. To master the material growth under various forms (2D film, 3D structures, nanostructures); and to develop and control the growth of new materials (whatever the epitaxial technique), **it is essential to understand the fundamental mechanisms driving their synthesis by closely combining theoretical and experimental approaches.**

We would like to express our thanks to all the organizing, technical program, and scientific committee members who worked to make this workshop a success.

All committee members are happy to meet you in Madrid.

Workshop Chairs

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April 19, 2023

12h00	**Registration**
14h00	**Welcome & Workshop opening**
14h30	*S1.01* - **M. Milanović -** *Invited Speaker* Polymer assisted deposition technique: a chemical solution route to high quality LaMnO3 thin films
15h00	*S1.02* - **R. Butkutė -** Complex study of processes in Ga(As,Bi)/(Al,Ga)As quantum structures Initiated by in-situ MBE annealing
15h15	*S1.03* - **A. Mahmoudi -** Electronic band structure of CVD-grown two-dimensional rhombohedral
15h30	*S1.04* - **F. Hensling -** Homoepitaxial growth of c-plane sapphire of unmatched quality by thermal laser epitaxy
15h45	*S1.05* - **C. Chirila -** Hafnia based epitaxial nanolaminates
16h00	**Coffee Break**
16h45	*S2.01* - **P. Żabiński -** The role of epitaxial layer of oxides on surface of hydrogen evolution electrocatalyst
17h00	*S2.02* - **S. Kret -** TEM analysis of semi-coherent epitaxial shells of semiconductor nanowires grown by MBE
17h15	*S2.03* - **N. Shepelin -** Insights into the growth of coherent Ag(Nb,Ta)O3 thin films
17h30	*S2.04* - **M. Toda i Casaban -** Epitaxial growth of perovskite manganite thin films by polymer assisted deposition for spintronic applications
17h45	*S2.05* - **P. Dziawa -** MBE grown GaAs-Pb(1-x)Sn(x)Te Core-Shell Nanowires
18h00	*S2.06* - **D. Y. Kim -** Growth of Oxide and Nitride Thin Films by Thermal Laser Epitaxy
18h15	*S2.07* - **S. Stanionytė -** MBE growth and structural characterization of thin bismuth layers

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April 20, 2023

8h00	**Registration**
8h30	*S3.01* - **E. Dudutienė -** Growth and optical properties of GaAsBi quantum wells with parabolic AlGaAs barriers
8h45	*S3.02* - **J. Sadowski -** TaAs Weyl semimetal thin films grown by molecular beam epitaxy
9h00	*S3.03* - **J. P. B. Silva -** Ferroelectricity in epitaxial ZrO2 thin films
9h15	*S3.04* - **E. Işık -** Electrical Characterization of Fullerene (C70) - TiO2 Nanotubes Heterostructure
9h30	*S3.05* - **S. Chen -** Microstructure and Magnetization Dynamics in La2/3Sr1/3MnO3 Epitaxial Thin Films
9h45	*S3.06* - **L. Pellegrino -** Pulsed laser deposition of LaAlO3 films for MEMS applications
10h00	*S3.07* - **H. Şahin -** Experimental and Theoretical Investigation of the Usability of Graphene-like 2D Crystals in Chemical Sensor Applications
10h15	**Coffee Break**
11h00	*S4.01* - **Vesselin Tonchev** - *Invited Speaker* The Pimpinelli Tonchev Videcoq Vladimirova (PTVV) theory: 21 years after
11h30	*S4.02* - **J-N. Aqua -** Growth mechanisms of 2D materials: the Kinetic Monte-Carlo point of view
11h45	*S4.03* - **V. Deibuk -** Phase Stability of Thermoelectric ZnSb-SnTe Thin Films
12h00	*S4.04* - **J. Johansson -** Understanding Kinking of Semiconductor Nanowires
12h15	*S4.05* - **C. Cornet -** Wetting properties of heteroepitaxial systems determined from surface and interface energies calculations
12h30	**Lunch**
14h00	*S5.01* - **C. Barbot -** Selective Area Growth of in-plane In0.5Ga0.5P nanowires on GaAs(111)B substrate by molecular beam epitaxy
14h15	*S5.02* - **M. Alonso -** MBE growth of Si-based nanocrystal pyramids on pit-patterned Si(001)
14h30	*S5.03* - **A. Kaleta -** MBE-grown nanowires with wurtzite GaAs cores and ferromagnetic shells investigated by scanning transmission electron microscopy
14h45	*S5.04* - **E. Butanovs -** Growth of few-layer van der Waals materials on semiconductor nanowires
15h00	*S5.05* - **S. KANG -** Growth and NMR study of high quality ordered Mn5(Six Ge1-x)3 thin films on Ge(111) substrate
15h15	*S5.06* - **N. Chapuis -** Key parameters for GaP(111)B surface preparation and Selenium passivation
15h30 - 18h00	**Coffee Break & Poster session**

April 21, 2023

8h00	**Registration**
8h30	*S6.01* - **S. Calcaterra -** Germanium Quantum Wells for Spin Qubit Applications
8h45	*S6.02* - **R. Vilarinho -** Electric-field engineered lattice distortions for optoelectronic devices
9h00	*S6.03* - **Q. Hochart -** Combining Molecular Beam Epitaxy and Metal-Organic Chemical Vapor Deposition for GaInAsP-based Ultra-Wide Band Semiconductor Optical Amplifiers for device's performance optimization
9h15	*S6.04* - **D. Dimitrov -** Study on the epitaxial growth of WSe2 on PtSe2 sublayer
9h30	*S6.05* - **T. Malinauskas -** Remote Epitaxy of GaN via Graphene on GaN/Sapphire Templates
9h45	*S6.06* - **M. Kolibal** - *Invited Speaker*
10h00	In-situ microscopy: Phase transformations during phosphorene formation on Cu(111)
10h15	**Coffee Break**
11h00	*S7.01* - **M. Melo Nogueira Rosa Gomes -** The role of structural distortions in triggering the metal to insulator transition in NdNiO3
11h15	*S7.02* - **L. Vincent -** Epitaxy of hexagonal Ge-2H: growth regimes and related I3 defects
11h30	*S7.03* - **G. Bell -** Molecular Beam Epitaxial Growth of SrMnSb2 Thin Films
11h45	*S7.04* - **T. Musálek -** Congruent evaporation of CsPbBr3 perovskite studied by Knudsen Evaporation Mass Spectroscopy
12h00	**End - few words**
12h15	
14h00 - 15h30	**Lab Tour**

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Polymer assisted deposition technique: a chemical solution route to high quality $LaMnO_3$ thin films

Marija Milanović[1*], Jelena Vukmirović[1], Sara Joksović[2], Danica Piper[1], Andrea Lazić[1], Mirjana Novaković[3], Vladimir V. Srdić[1]

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Keywords: $LaMnO_3$, thin films, PAD

Thin films play an important role in the development of microelectronics. They offer a huge contribution in lower consumption of energy and materials, thus improving the performance of electronic devices. Transition metal oxides with perovskite structures exhibit a variety of unusual properties including ferromagnetism, ferroelectricity, giant/colossal magnetoresistance effects and multiferroics (simultaneous ferroelectricity and ferromagnetism), making them excellent candidates for various devices applied in electronics and sensors [1]. In particular, lanthanum manganite based thin films are recognized as a good material for those applications. To obtain high quality epitaxial ceramic thin film, often requires the usage of sophisticated and expensive equipment. Searching for environmentally friendly and low-cost deposition method have led to development of polymer assisted deposition technique (PAD). In comparison to the vapor deposition methods, PAD is simple, economic technique with a good control of stoichiometry and with a high throughput large-scale production.

In this work, $LaMnO_3$ based thin films were prepared by PAD technique and deposited at different single crystal substrates in order to investigate the possibility of their epitaxial growth from a liquid phase. Stoichiometric amounts of metal cations were dissolved in distilled water with the addition of water-soluble polymers EDTA and PEI used as complexation agents. In order to find the optimal rheological parameters for deposition of thin films, the concentration of the metal solutions as well as the amount of the used polymers were varied. Optimization of process parameters and selection of appropriate substrate play an important role in preparation of epitaxial structures, since matching of the unit cell of substrate and the film is crucial for the preferential growth and high quality of the film. The prepared solutions were spin coated onto substrates and thermally treated at different temperatures up to 900°C in order to produce $LaMnO_3$ based films. The thickness of the film can be easily controlled by the concentration of precursor and the coating speed. Structure and phase composition is examined by X-ray diffraction analysis, while the thickness and the formation of the epitaxial films were observed using transmission electron microscopy. The results have confirmed that epitaxial $LaMnO_3$ based thin films were successfully prepared by PAD on different single crystal substrates.

References:

1. H. Liu et al., Surface & Coatings Technology 226 (2013) 108–112

Complex study of processes in Ga(As,Bi)/(Al,Ga)As quantum structures initiated by *in-situ* MBE annealing

Arnas Pukinskas, Arnas Naujokaitis, Martynas Skapas, Sandra Stanionytė, Monika Jokubauskaitė, Bronislovas Čechavičius, Evelina Dudutienė and Renata Butkutė*

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Keywords: bismide, NIR, quantum structure, MBE, *in situ* annealing, HR-XRD, HR-TEM, STEM, PL

The engineering of new materials and scale-reduction of the objectives have attracted a lot of attention of scientific community in the last decade. Our previous investigations demonstrated variety of technological protocols, including change of the quantum well design, pauses in epitaxy, annealing processes, serving for the smoothing of interfaces, atom diffusion, improvement of the crystalline quality and reduction of density of defects as well for enhancement of electrical or optical properties [1-4]. Moreover, the new epitaxy methods using modified substrate surface or droplet-initiated processes could lead to the achievement of flexible functional materials and nanostructures. Thus likely, the integration of both quantum effects and new epitaxial approaches supposes to reach the technological synergy, which opens new possibilities for manipulation by structural and physical properties of semiconductor nanostructures.

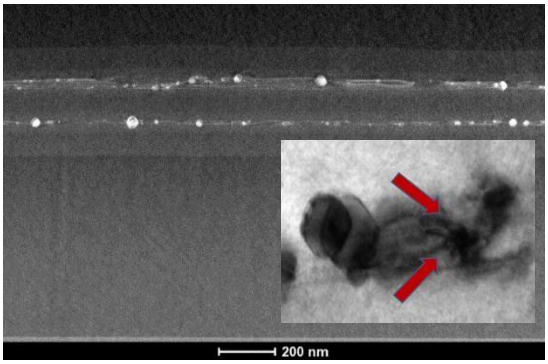

Fig. HR-TEM image of Ga(As,Bi)/(Al,Ga)As MQW, annealed at 700°C for 90 s. The inset shows Bi segregation channels.

The goal of this investigation was to explore and understand the processes in Ga(As,Bi)/(Al,Ga)As quantum wells initiated by *in situ* annealing in MBE rector. To explore this, the multiple quantum wells (MQW) of Ga(As,Bi)/(Al,Ga)As were grown at low temperatures (370°C – 425°C) using solid source Molecular Beam Epitaxy (MBE). Further, thermal treatment of bismide-based MQW structures was performed *in situ* in MBE reactor by annealing in the temperature range of 550°C÷750°C for 60 s ÷ 180 s. All samples were characterized using high resolution Xray diffraction (HR-XRD), transmission electron microscopy (HR-TEM) and photoluminescence (PL) measurements.

The obtained results defined the relationship between MQW growth and *in situ* annealing conditions. It was determined that quantum barrier composition (which could play Bi blocking layer role), well composition and design (well thickness and shape) influence Bi atoms diffusion in and out of the well. The detailed analysis of HR-TEM images revealed temperature and time dependent Bi segregation dynamics (see Figure).

This research was supported by Research Council of Lithuania under the grant No. S-MIP-22-86 (LMTLT).

[1] R. Butkutė et al., Thermal annealing effect on the properties of GaBiAs, Phys. Status Solidi C 9, No. 7, 1614– 1616 (2012).
[2] R. Butkutė et al., Migration-Enhanced Epitaxy of Thin GaAsBi layers, Lith. J. Phys., Vol. 54 No. 2, pp. 125–129 (2014).
[3] R. Butkutė et al., Bismuth quantum dots in annealed GaAsBi/AlAs quantum wells, Nanoscale research letters 12 (1), 436, 3 (2017).
[4] S Pūkienė et al., Enhancement of photoluminescence of GaAsBi quantum wells by parabolic design of AlGaAs barriers, Nanotechnology, Vol. 30, 455001 (11pp) (2019).

Electronic band structure of CVD-grown two-dimensional rhombohedral WSe_2 homobilayers

Aymen Mahmoudi*[1], Geoffroy Kremer[1], Julien Chaste[1], Pavel Dubin[2], José Avila[2], Fabrice Oehler[1], Abdelkarim Ouerghi[1]

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Keywords: CVD, 2D, Raman, ARPES

Twisted layers of atomically thin two-dimensional materials realize a broad range of novel quantum materials with engineered optical and transport phenomena arising from spin and valley degrees of freedom and strong electron correlations in hybridized interlayer bands[1,2]. Here, we report experimental and theoretical studies of WSe_2 homobilayers obtained in stable configurations of 2H (60° twist) and 3R (0° twist) stackings by controlled chemical vapor synthesis of high-quality large-area crystals[3,4,5]. We directly reported the electronic and structural properties of bilayer WSe_2 with the two stacking orders using micro-Photoluminescence (μ-PL) and micro-Raman spectroscopy, angle-resolved photoemission spectroscopy measurements (ARPES), and Density Functional Theory (DFT) calculations. Nano-ARPES clearly demonstrated that our bilayer with AB stacking shows a high spinorbit coupling of about 550 meV. Our work opens up new perspectives in the development of optoelectronic and spintronic devices made of easily processable TMDs materials.

References

[1] Ruitao Lv et al. Acc. Chem. Res. 2015, 48 (1), 56–64. [2]
G. Wang et al, Rev. Mod. Phys. 90, 3721 (2018).
[3] Jiangang He, et al. Phys. Rev. B 89, 075409 (2014)
[4] Zhijie Li et al. Phys. Rev. B 106, 045411 (2022) [5]
K. M. McCreary et al. Nanoscale 14, 147 (2022).

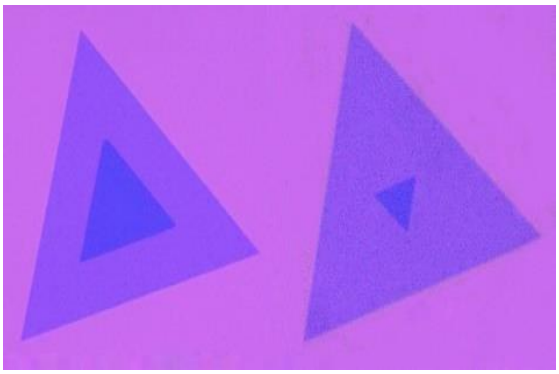

Figure 1: Optical image of CVD-grown WSe_2 bilayer flakes

Homoepitaxial growth of c-plane sapphire of unmatched quality by thermal laser epitaxy

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Keywords: Oxides, Innovation, ultra-wide bandgap, substrate preperation, high power electronics

The interest in sapphire as an electronic material is due to its low cost, superior properties over silicon, high quality wafer availability, and the possible integration with silicon. Indeed, its rapidly growing market share suggests sapphire to be the substrate material of the future.[1] A cornerstone for further establishing sapphire in a wide range of (electronic) applications is the ability to grow high quality homoepitaxial sapphire films. Key applications that can benefit from this are, *e.g.* nitrides for diode applications,[1] and (ultra) wide band gap semiconductors for high power electronics.[2,3] However, even the best molecular-beam epitaxy films of sapphire on sapphire to date lack the atomic smoothness and purity desired for many applications.[3] The underlying reasons are the difficult handling of aluminium effusion cells in oxygen atmospheres, and the desirable substrate temperatures which are so high that they are hard to reach with conventional substrate heaters.
The recent development of thermal laser epitaxy (TLE), however, promises the availability of a parameter space far exceeding other deposition methods.[4] I will present how TLE is able to overcome the issues associated with the homoepitaxial deposition of sapphire. The uniqueness of a freestanding source with very localized heating avoids any contaminations from crucibles and any flux drift from undesired source oxidization. The substrate laser heating system allows to easily heat sapphire substrates even beyond their melting point. This enables a precise and smooth sapphire substrate preparation – the first step for successful homoepitaxy.[5] I further present how the crystal quality and surface smoothness of homoepitaxial sapphire increase with increasing substrate temperature. Films were investigated by scanning transmission electron microscopy, atomic force microscopy, and x-ray diffraction. At a growth temperature of 1600 °C they were found to be practically undistinguishable from the underlying substrate.

References

[1] M.S. Akselrod, F.J. Bruni, "Modern trends in crystal growth and new applications of sapphire," *J. Cryst. Growth*, 360, pp. 134-145, 2012.
[2] H. Okumura, "Sn and Si doping of α-Al_2O_3 (10-10) layers grown by plasma-assisted molecular beam epitaxy", *JJAP*, 61, 125505, 2022.
[3] R. Jinno *et al.*, "Crystal orientation dictated epitaxy of ultrawide-bandgap 5.4- to 8.6-eV α-$(AlGa)_2O_3$ on m-plane sapphire", *Sci. Adv.,* 7, eabd5891, 2021
[4] W. Braun and J. Mannhart, "Film deposition by thermal laser evaporation," *AIP Advances,* 9, 085310, 2019.
[5] W. Braun *et al.*, "*In situ* thermal preparation of oxide surfaces", *APL Mater.,* 8, 071112, 2020.

Hafnia based epitaxial nanolaminates

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Keywords: epitaxy, hafnia, nanolaminates

Here we report the growtht and characterization of complex nanolaminate structures based on HfO_2 materials. In the last years a significant number publications reported different deposition methods used to stabilize the ferroelectric phase of HfO_2 by doping or by substrate changing [1-3]. Recently, large radius dopant atoms as La, have gained more scientific attention. High values of polarization and endurance have been reported on 2% or 5% La content [4]. On polycrystalline nanolaminates, artificially induced antiferroelectricity has recently been reported using HfO_2/ZrO_2. These findings demonstrate the potential of this materials for the energy storage area, but there are significant issues that need to be addressed. The aim of this study was to comprehend if the antiferroelectricity can be artificially created in epitaxial nanolaminates obtained from HfO_2 dopped with 5% La (HLO), as ferroelectric and ZrO_2 (ZO) as dielectric materials. Epitaxial capacitors from HLO/ZrO_2 nanolaminate layers were grown by pulsed laser deposition (PLD) on (001) and (110)-oriented single crystalline $SrTiO_3$ (STO) substrates with $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) bottom electrode. Different configurations of ferroelectric/dielectric were tested: asymmetric configuration where a dielectric is deposited between the ferroelectric layer and one of the electrodes; symmetric configurations where the dielectric is placed between two ferroelectric layers or with ferroelectric placed between two dielectric layers. The influence of the ratio between the thicknesses of the ferroelectric/dielectric on the ferroelectric phase formation and electrical properties were also investigated. The structural properties investigated by X-ray diffraction with a 1D and 2D detectors revealed the stabilization of ferroelectric phase. The polarization loops with specific switching current characteristics also confirm the ferroelectric behaviour of the epitaxial nanolaminates. Obtained results on epitaxial nanolaminate structures do not confirm the presence of the antiferroelectric behavior like was reported for the case of the polycrystalline nanolaminates.

References:

1. Tingfeng Song, et al., Improved polarization and endurance in ferroelectric Hf0.5Zr0.5O2 films on SrTiO3(110), Nanoscale, 14, 6 (2022)
2. H. Alex Hsain, et al., The Many Routes to Ferroelectric HfO2: A Review of Current Deposition Methods, Journal of Vacuum Science & Technology A **40**, 010803 (2022)
3. J.P.B. Silva, et al., Progress and perspective on different strategies to achieve wake-up-free ferroelectric hafnia and zirconia-based thin films, Applied Materials Today 26, 101394 (2022)
4. Tingfeng Song, et al., Impact of La Concentration on Ferroelectricity of La-Doped HfO2 Epitaxial Thin Films ACS Appl. Electron. Mater. 3, 4809−4816 (2021)

The role of epitaxial layer of oxides on surface of hydrogen evolution electrocatalyst

Katarzyna Skibińska[1], Konrad Wojtaszek[1], Lukas Krause[2], Anna Kula[1], XuegengYang[3], Mateusz M. Marzec[4], Marek Wojnicki[1], Piotr Żabiński[1*]

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Keywords: electrocatalysis, hydrogen evolution reaction, epitaxial oxide layer, controlled oxidation

Catalysts can be successfully prepared by a simple electrochemical process. Their surface composition distinguishes catalytic activity toward hydrogen or oxygen evolution reactions. In this work, uniform Co-Ni cones were synthesized using the one-step method from an electrolyte containing a crystal modifier. Electrodeposited layers were oxidized and/or reduced in the furnace at 100°C. Freshly electrodeposited coating was stored in air atmosphere for seven days. This results in an epitaxial oxide layer forming on the surface of the catalyst. Changes in the surface composition, confirmed by the XPS method, strongly influenced the wettability, catalytic performance, and size of evolved hydrogen bubbles. The conical Co-Ni surface with epitaxial oxides layer formed in a controlled way possesses the best catalytic activity towards hydrogen and oxygen evolution. Conversely, the spontaneously formed oxide layer decreases the catalytic performance in mentioned reactions compared with the fresh sample. That open a possibility to control electrocatalytical activity of material by proper grow of thin layer of oxides. The proper storage of synthesized samples is also essential due to their desired catalytic applications. Proposed controlled oxidation can be an accessible way to increase nanomaterials catalytic performance.

TEM analysis of semi-coherent epitaxial shells of semiconductor nanowires grown by MBE.

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Keywords: nanowires, plastic relaxation, dislocations, MBE, HRSTEM, strain

Due to the high surface-to-volume ratio, the monocrystalline semiconductor core-shell nanowires (NW) are very attractive as building blocks of solar cells, and optoelectronic, electronic, and environmental sensor devices. They are also perfect model structures for investigating the nanomechanical behavior of defects appearing during strain relaxation. We study two semiconductor radial NW heterostructures: the first one based on wurtzite (hexagonal) (In,Ga)As, the second one on cubic (Cd,Zn)Te. Dislocations in individual NWs, are investigated in two configurations: (i) plan view – NWs lying on a TEM grid; (ii) cross-sectional view - thin NW slice cut in the direction perpendicular to NW axis. The focused ion beam (FIB) technique has achieved the letter. The Dislocation Density Tensor mapping was realized using an extension of the Geometric Phase Analysis [1] performed on High-Resolution (HR) TEM and HR-STEM images of both specimen types at different zone axes. In the case of NWs with CdTe core, the stress relaxation occurs by creating a misfit dislocations network at the core-shell interface consisting of 60° dislocations and dissociated Lomer dislocations. We show that axial and radial spacing between dislocations depends strongly on the local shell thickness and on the core diameter Fig1. These findings are in qualitative agreement with the theoretical predictions [2] and molecular dynamics simulations based on BOB, interatomic potential implemented in LAMMPS [3]. Additionally, we found a fundamental difference in the defect types in the case of the NWs with ZnTe core and CdTe shell. The basal plane Stacking Faults (SFs) or twin boundary of the core, interact with the (-111) plane SFs formed in the Cd-rich shell which results in the formation of partial dislocations (Cottrell-Lomer lock and Hirth lock) at the intersection of this these two sets of SFs. The plastic relaxation of the (Ga,In)As hetero-NWs occurs by the creation of misfit dislocations loops, (MDLs) around the core, which are not regularly spaced in an axial direction. We conclude that the observed difference in the mechanism of strain relaxation depends on the type of crystal structure (wurtzite or zinc blende) and the specific energy of defect formation.

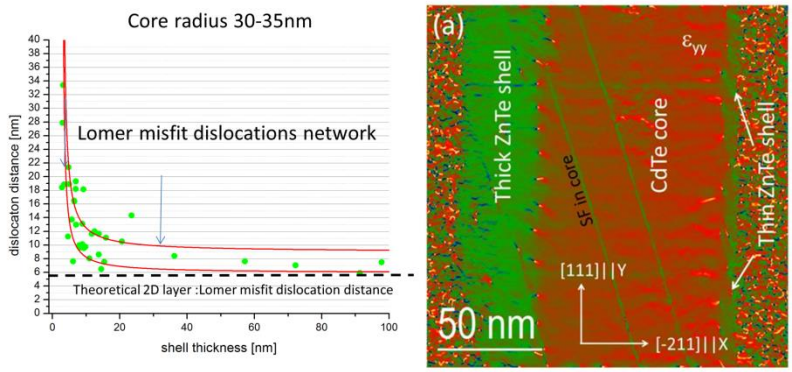

Fig. GPA determined map of ε_{yy} component of residual strain for CdTe nanowire with asymmetric ZnTe shell; The distance between misfit dislocations as well as degree of relaxation depends on the shell thickness.

[1] S. Kret, et. al (2003) Philos. Mag.83, 231
[2] O. Salehzadeh et.al (2013), J. Appl. Phys., 114 (5) (2013)
[3] D. K. Ward, et.al, Phys. Rev. B 85, 115206

Insights into the growth of coherent $Ag(Nb,Ta)O_3$ thin films

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Keywords: antiferroelectric, strain engineering, dielectric capacitor

The utilization of non-linear dielectric materials in energy storage is a topic of widespread recent research interest. Relaxor ferroelectrics and antiferroelectrics show favorable properties for this application, including a large recoverable energy density and a high electrical efficiency. While the optimally performing material compositions for energy storage contain lead, recent research has demonstrated the possibility of utilizing $Ag(Nb,Ta)O_3$ (ANT) as a lead-free substitute. ANT is a solid solution containing $AgNbO_3$ and $AgTaO_3$, whereby the former exhibits antiferroelectricity and the latter exhibits relaxor-like properties. Thus, the B site cation ratio enables the modulation of non-linear behavior in ANT. Studies in polycrystalline powder systems have demonstrated a recoverable energy density of 6.3 J cm^{-3} and an efficiency of 90% at room temperature for an optimized composition of $Ag(Nb_{0.5}Ta_{0.5})O_3$.[1] Therefore, it is an excellent candidate for thin film studies. In particular, the coherent growth of ANT under biaxial strain is a possible pathway to further increase the recoverable energy.

ANT is a complex material system, with the A site cation exhibiting significantly higher volatility relative to the B site, which results in Ag deficiency for ANT films grown by pulsed laser deposition (PLD). One recent study has reported epitaxial $AgNbO_3$ films grown by PLD, showing a rocking curve full width half maximum of 0.5° and demonstrating antiferroelectric behavior along the c axis.[2] This work shows great promise for tailoring relaxor antiferroelectric behavior through Ta incorporation and further enhancements due to strain engineering.

Here, we present for the first time the optimization of coherent growth for ANT thin films by PLD on oxide substrates with biaxial strain values up to 2.4%. We demonstrate the insights obtained during *in situ* monitoring of the evolution of the growth mode (high-pressure reflection high-energy electron diffraction, RHEED) and stress (multi-beam optical stress sensor, MOSS). This data is complemented by the *ex situ* analysis utilizing X-ray diffractometry and electron microscopy, correlating the real-time information to the structural and chemical properties. We further discuss the role of Ag excess in the target and its influence on the film composition towards achieving stoichiometric ANT thin films with a robust antiferroelectric response. Finally, we discuss the possibilities for dielectric and ferroelectric properties in strain-engineered ANT films in the ultra-thin regime.

1. N. Luo *et al.*, *Nature Communications*, **11,** 4824 (2020).
2. Y. Zhang *et al.*, *Journal of Materiomics*, **7,** 1294-1300 (2021).

Epitaxial growth of perovskite manganite thin films by polymer assisted deposition for spintronic applications

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Keywords: Polymer-assisted deposition (PAD); Lanthanum strontium manganite, Spintronics

Lanthanum strontium manganite ($La_{1-x}Sr_xMnO_3$) is a perovskite oxide with a huge appeal because of its wide variety of electronic and magnetic properties, such as colossal magnetoresistance, halfmetallicity, and metal-insulator transitions [1], which can be tuned by Sr doping level, as it is responsible for Mn ions valence [2]. Epitaxial $La_{1-x}Sr_xMnO_3$ thin films with high-quality, well-oriented, with minimal structural and chemical imperfections are desired. The polymer-assisted deposition (PAD) technique was chosen among the different grown methods, as it is a promising methodology with environmentally friendly, low-cost scalability and stoichiometric versatility [3].

Taking advantage of the PAD's stoichiometric versatility, epitaxial oxide $La_{1-x}Sr_xMnO_3$ thin films, with $0.3 \leq x \leq 0.65$, were grown on top of single crystalline (001)-$SrTiO_3$ substrates. Flat and fully strained $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) epitaxial thin films could be obtained with the expected ferromagnetic behaviour (T_c = 340 K). In addition to the characteristic resonant peaks that these films displayed when characterized by ferromagnetic resonance, LSMO films also evidenced a spin-pumping effect when a Pt film was deposited on top of it (see Figure 1). Thus, PAD demonstrated its efficiency in growing high quality LSMO epitaxial films for spintronic applications.

$La_{1-x}Sr_xMnO_3$ thin films with $x \geq 0.5$ were grown to use its A-type antiferromagnetic (AF) behaviour to improve the spin injection from a ferromagnet into a normal metal [4]. However, it was necessary to reach a doping level of 0.65 to get the expected Mn^{3+}:Mn^{4+} ratio according to XAS study. $La_{0.35}Sr_{0.65}MnO_3$ thin films should have ferromagnetic ordering planes, which are coupled antiferromagnetically, thus resulting in transport anisotropy along these films.

References

[1] Salamon, M. B., Rev. Mod. Phys., **73**, 583 (2001)
[2] Tokura, Y., *Reports Prog. Phys*, **69**, 797-851 (2006)
[3] Jia, Q; et. al., *Nat. Mater*., **3**, 529-532 (2004)
[4] Wang H.; et. al., *Phys. Rev. B*, **91**, 220410 (2015)

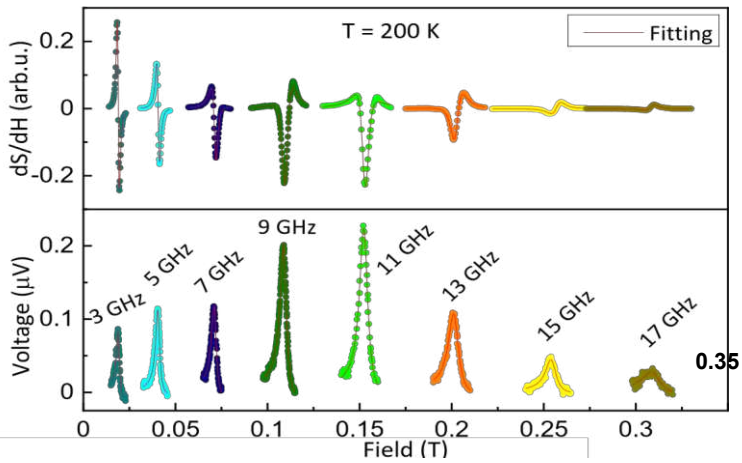

Figure 1: FMR spectra and Inverse Spin Hall voltage signal as a function of applied magnetic field, measured at 200 K for different frequencies in the Pt/LSMO/STO system.

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MBE grown GaAs-Pb(1-x)Sn(x)Te Core-Shell Nanowires

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Keywords: nanowires, topological crystalline insulators, core-shell

Abstract
Layered heteroepitaxial systems usually face the problem of thermal and lattice misfit of their individual components. Stacking of dissimilar materials usually generates strain and can result in a high density defects located at the interface and within the layers constituting the heterostructure. One-dimensional systems, such as nanowires (NWs), offer the possibility to reduce this effect by accommodating stresses between the heterostructure constituents [1]. We use a combination of GaAs and Pb(1-x)Sn(x)Te semiconductor materials with relatively high mismatch of the bulks (above 12%),. We exploit the coreshell nanostructure where the core is constituted by wurtzite GaAs NW and the shell is made with Pb(1-x)Sn(x)Te IV-VI semiconductor. In such configuration the lattice mismatch along the [001] WZ GaAs NW core is much less (below 4%) than the bulk one. We show that it is possible to grow Pb(1-x)Sn(x)Te shells in two distinct orientations (100) or (110). Applying Pb(1-x)Sn(x)Te which is known to be a topological crystalline insulator brings an extra degree of freedom to modify its electronic properties due to the chemical composition and/or temperature dependent topological phase transition [2]. This transition can also be controlled by pressure [3] and strain - as in the (III-V)-(IV-VI) epitaxial heterostructures studied by us. Contrary to the NWs perpendicular to the surface the use of inclined nanowires makes it possible to grow half-shells which allows to access and investigate 1D NW edges, possibly exploiting also the 1D higher order topological insulator states, theoretically predicted for some IV-VI narrow gap semiconductors [4].

Acknowledgments
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References
[1] E. Ertekin, P.A. Greaney, D. Chrzan, T.D. Sands, Equilibrium limits of coherency in strained nanowire heterostructures, Journal of Applied Physics 97 (2005) 114325.
[2] S.-Y. Xu, et. al., Observation of a topological crystalline insulator phase and topological phase transition in Pb1− xSnxTe, Nature communications 3 (2012) 1-11.
[3] P. Barone, T. Rauch, D. D. Sante, J. Henk, I. Mertig, S. Picozzi, Pressure-induced topological phase transitions in rocksalt chalcogenides, Physical Review B 88 (2013): 045207.
[4] F. Schindler, A. M. Cook, M. G. Vergniory, Z. Wang, S. S. P. Parkin, B. A Bernevig and T. Neupert, Higher-order topological insulators, Sci. Adv. 4 (2018) eaat0346Abstract (Calibri, 11, 1-page max including eventual illustrations)

Growth of Oxide and Nitride Thin Films by Thermal Laser Epitaxy

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Keywords: Epitaxy, Thermal laser epitaxy, Metal oxides, III-nitrides, high-temperature growth

Abstract

Thermal laser epitaxy (TLE) is a novel film growth technique that uses continuous-wave laser beams to thermally vaporize pure elemental sources and to heat substrates in almost any background atmosphere to nominally unlimited temperatures [1]. TLE eliminates the need for heaters operated inside the deposition chamber while benefiting from the deposition modes of molecular beam epitaxy and chemical vapor deposition.
The possibility to use a wide range of source elements [2], extreme substrate temperatures [3], and deposition in high-pressure atmospheres of reactive gases [4] makes TLE suitable for the growth of oxide and nitride thin films under extreme conditions.
In this presentation, we describe the operation principles of TLE and its advantages based on using continuous-wave lasers as power sources. We have been successful in growing a spectrum of binary oxide thin films by evaporating pure elemental sources in oxygen atmospheres, and III-nitride thin films in nitriding atmospheres produced by plasma-induced free N radical or NH_3 gas sources.
Our results reveal the potential of TLE in handling any elemental sources including refractory metals for epitaxial film growth. They open up new possibilities for the epitaxial growth of transition metal nitrides and ultrahigh-purity heterostructures that comprise very diverse materials systems.

References

[1] W. Braun and J. Mannhart, *AIP Adv.* **9**, 085310 (2019)
[2] W. Braun, M. Jäger, G. Laskin, P. Ngabonziza, W. Voesch, P. Wittlich and J. Mannhart, *APL Mater.* **8**, 071112 (2020)
[3] T. J. Smart, J. Mannhart and W. Braun, *J. Laser Appl.* **33**, 022008 (2021)
[4] D. Y. Kim, J. Mannhart and W. Braun, *APL Mater.* **9**, 081105 (2021)

MBE growth and structural characterization of thin bismuth layers

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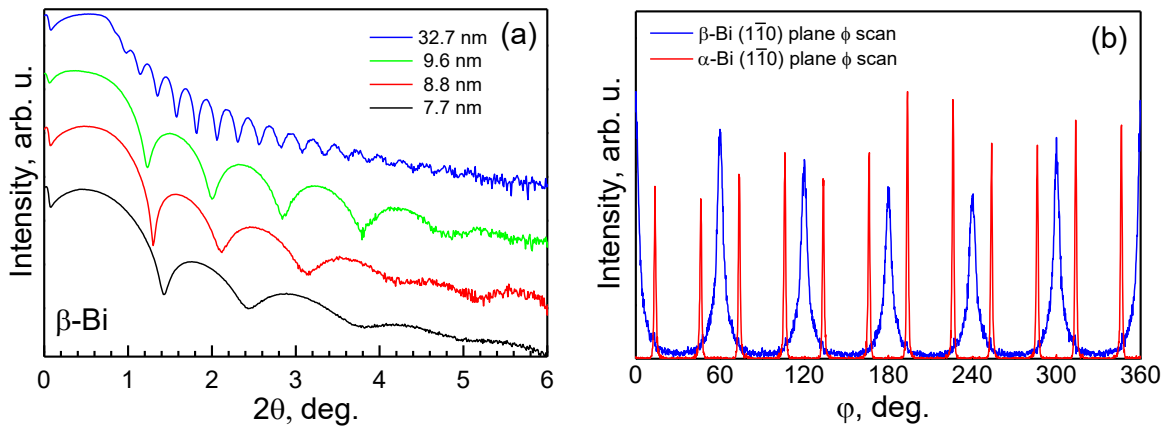
Keywords: 2D bismuth, X-ray reflectivity, X-ray diffraction, in-plane measurements

Thin Bi layers attract attention as promising candidates for 2D topological insulators. In layers thinned down to ~30 nm semimetal to semiconductor transition is obtained and, moreover, layers grown Si substrates could be easily compatible with existing silicon technology.

In this work, thin layers of bismuth were grown on Si (111) substrates by molecular beam epitaxy (MBE) varying different growth parameters. Bulk bismuth has a rhombohedral structure, but depending on growth temperature, thin layers of Bi can be grown in different orientations – (111)-oriented (β-Bi) and (110)-oriented (α-Bi).

The thicknesses of analyzed samples were calculated from X-ray reflectivity measurements and varied from 6 up to 30 nm (Fig. 1a). The orientations of Bi films were identified from out-of-plane and in-plane (Fig. 1b) X-ray diffraction measurements. Analyzing the relation between growth orientation and growth condition it was revealed that β-Bi formation prefers higher growth temperatures. Layers are homogenous, have hexagonal symmetry in growth direction. They are biaxially compressed in the layer plane and tensile in the growth direction. Meanwhile α-Bi layers which are tend to form at lower growth temperatures have several in plane orientations, insets of β-Bi and are compressively strained. Both types of strains decrease with increasing layer thickness.



1 pav. (a) X-ray reflectivity measurements of different β-Bi films; (b) In-plane relation between α-Bi and β-Bi planes perpendicular to surface.

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Growth and optical properties of GaAsBi quantum wells with parabolic AlGaAs barriers

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Keywords: GaAsBi, parabolic quantum well, quantum dots, carrier localization, MBE

The main weaknesses of semiconductor quantum structure based infrared lasers are temperaturedependent lasing wavelength and non-radiative losses due to Auger recombination. GaAsBi are relatively new compound with anomalously fast band gap reduction and temperature-insensitive bandgap. Moreover, large spin-orbit split-off energy, which exceeds the bandgap energy, when bismuth content is higher than 10 %, leads to effective non-radiative Auger recombination suppression [1]. However, the molecular beam epitaxy growth of high quality GaAsBi structures is complicated due to extremely low growth temperatures required for Bi incorporation and large radius of Bi atoms. Search of ways to increase PL intensity of GaAsBi quantum wells (QW) led to growth of unconventional parabolic AlGaAs barriers. It was shown that PL intensity of GaAsBi QW with parabolic barriers increased more than 50 times. Moreover, enhanced PL intensity of parabolic GaAsBi QW is reproducible over the growth conditions [2]. Even more increased PL intensity was expected by growing multiple GaAsBi/GaAs/AlGaAs QWs. Different types of parabolic AlGaAs barrier designs were grown and investigated (see Fig. 1). It was demonstrated that design of parabolic AlGaAs barrier unaffected the emission wavelength of GaAsBi at room temperature. On the other hand, relation between PL intensity and barrier type was observed. Finally, thermal annealing effect on GaAsBi/GaAs/AlGaAs QWs was investigated. It was shown that *in situ* annealing for 3 min at 750 °C (substrate temperature) led to structural and optical changes of the GaAsBi samples, observed in transmission electron microscopy images and photoluminescence spectra.

This research was supported by Research Council of Lithuania under the grant No. S-MIP-22-86 (LMTLT).

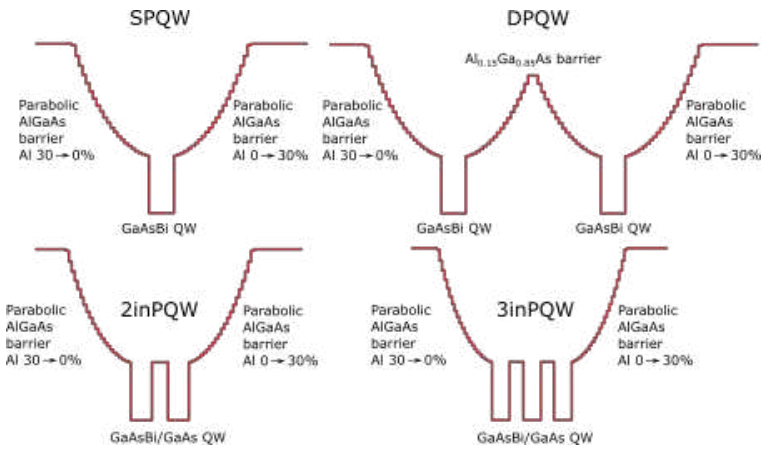

Fig. 1. Types of GaAsBi/GaAs/AlGaAs multiple-quantum well designs.

[1] Usman, Muhammad, et al. "Tight-binding analysis of the electronic structure of dilute bismide alloys of GaP and GaAs." Physical Review B 84.24 (2011): 245202.
[2] Pūkienė, S., et al. "Enhancement of photoluminescence of GaAsBi quantum wells by parabolic design of AlGaAs barriers." Nanotechnology 30.45 (2019): 455001.

TaAs Weyl semimetal thin films grown by molecular beam epitaxy

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Keywords: MBE growth, Weyl semimetals

TaAs is the first experimentally realized topological Weyl semimetal (WSM) [1]. Until recently it has only been studied in the form of bulk crystals (after cleaving or cutting thin slices, depending on the type of subsequent measurements [1-2]). Similar to other WSM materials, due to a distinct electronic structure TaAs exhibits unique magnetotransport properties, such as giant anisotropic magnetoresistance - positive or negative, depending on the mutual orientation between electric and magnetic fields, with respect to the TaAs crystallographic directions. Recently we have shown, that thin, monocrystalline TaAs films can be grown by MBE on commonly used GaA(001) substrates [3]. This opens possibilities for integrating TaAs in heterostructures with magnetic materials (ferro- and/or antiferromagnets) enabling use of magnetic proximity effects instead of the external magnetic field.

TaAs layers have been grown in the SVTA III-V MBE system equipped with the e-beam source for Ta and valved cracker source for As. After depositing thin GaAs buffer layer on GaAs(001) epi-ready substrates, TaAs has been grown at the same conditions, i.e., at the substrate temperature of about 590 °C and As_2 flux the same as used for the GaAs buffer (As beam equilibrium pressure of about $5x10^{-7}$ mbar), with the TaAs growth rate of 1 ML /(10÷15) min. Interestingly in spite of a huge lattice mismatch between GaAs(001) and tetragonal TaAs (with the in-plane lattice parameter $a = b = 3.4368$ Å; and the perpendicular one $c = 11.6442$ Å) streaky 2D RHEED patterns were observed throughout the whole MBE growth starting from the deposition of the very first TaAs monolayer. The spacing of RHEED streaks also points to the TaAs film relaxation in the initial growth stage but neither 3D islanding, nor misfit dislocations at TaAs/GaAs(001) interface have been observed with *in-situ* RHEED and *ex-situ* transmission electron microscopy (TEM) investigations, respectively. X-ray diffraction (XRD) measurements confirm the complete relaxation of TaAs layers and indicate the 45 degrees in-plane rotation of TaAs(001) planes, with respect to the GaAs(001) substrate surface.

The atomic force microscopy measurements reveal the stripe-like TaAs surface morphology with about 20 nm wide and 200 nm long lateral stripes parallel to the [-110] GaAs crystallographic direction, keeping the same crystallographic orientation (as evidenced by XRD). For TaAs film thicknesses exceeding about 5 nm the stripes are merged together into continuous layer. The individual TaAs stripes have been investigated by scanning tunneling microscopy, using samples with protective amorphous As capping layers deposited directly after the MBE growth.

References

[1] Su-Yang Xu, I. Belpolski, et. al., and Zahid M. Hasan, Science, **349,** 613, (2015).
[2] Q. R. Zhang, et. al., Phys. Rev. B, **100**, 115138, (2019).
[3] J. Sadowski, et. al., Cryst. Growth Des. **22**, pp. 6039, (2022).

Ferroelectricity in epitaxial ZrO_2 thin films

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Keywords: ferroelectrics, zirconia, rhombohedral phase, charged defects, phase stability

Zirconia and hafnia based thin films have attracted considerable attention in the last decade due to the existence of a ferroelectric behavior at the nanoscale, which can enable the downscaling of the next-generation of non-volatile memory and energy storage devices [1-3].
The present work combines experimental studies with density-functional theory (DFT) calculations to disclose a novel polar rhombohedral R3m phase in epitaxially-strained (111)-oriented ZrO_2 thin films grown by ion-beam sputtering deposition technique on (111)-Nb:SrTiO3 substrates. In addition, we revealed the role of oxygen vacancies on the stability and ferroeletric polarization of these films, reaching 20.2 µC/cm2 with a coercive field of 1.5 MV/cm. Interestingly, the studied films show a ferroelectric behavior per se, i.e. a technological advantage over the previously studied conventional orthorhombic ZrO_2 films where a wake-up cycle process is usually needed to induce ferroelectricity [4].

[1] U. Schroeder, M. H. Park, T. Mikolajick, C. S. Hwang, Nat. Rev. Mat. 7, 653–669 (2022).
[2] J. P. B. Silva, K. C. Sekhar, H. Pan, J. L. MacManus-Driscoll, M. Pereira, ACS Energy Lett. 6, 2208–2217 (2021).
[3] S. S. Cheema, N. Shanker, S.-L. H. Rho, C.-H. Hsu, V. A. Stoica, Z. Zhang, J. W. Freeland, P. Shafer, C. P. Grigoropoulos, J. Ciston, S. Salahuddin, Science 376, 648–652 (2022).
[4] J P. B. Silva, R. F. Negrea, M. C. Istrate, S. Dutta, H. Aramberri, J. Íñiguez, F. G. Figueiras, C. Ghica, K. C. Sekhar, A. L. Kholkin, ACS Appl. Mater. Interfaces 13, 51383–51392 (2021).

Electrical Characterization of Fullerene (C_{70}) - TiO_2 Nanotubes Heterostructure

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TiO_2 is a semiconductor with various polymorphs that occur naturally or under high pressure and temperature, such as anatase, rutile and, brookite. It has wide range of applications in sensors [1], photovoltaic [2], photocatalysis [3], hydrogen production [4] and lithium batteries [5] due to its unique photoelectronic properties, high chemical stability, low cost, and minimal environmental impact. In order to create next-generation TiO_2 nanotubes based solid state gas sensors with improved structural, electrical, and chemical capabilities, nanocarbons have been extensively employed to functionalize various nanostructured materials. The carbon-based substance is one of the most researched and used materials in the nanotechnology area because of its exceptional features. When compared to other commonly used materials, carbonaceous structures have several advantages, particularly their exceptional physical-chemical characteristics. Carbon and graphene are the commonly used materials for the different kinds of nanostructure but fullerene has received very little attention. Carbon atoms are arranged in closed cage-like formations called fullerene molecules. The most well-known fullerene is C_{60}, which Krotoet discovered in 1985 [6]. C_{70}, another well-known molecule that was also identified in [6], is the second. The limited number of studies have been carried out on fullerene or fullerene-based nanocomposites for coating or decorating TiO_2 nanotubes.

In this study, the electrochemical anodization method was used to synthesize TiO_2 nanotubes by using high purity titanium foil as a substrate. The titanium foils were anodized at 40 V for 2 hours in the ethylene glycol based electrolyte. After anodization process, TiO_2 nanotubes were annealed at 500°C under dry air atmosphère. The annealed and as-growth TiO_2 nanotubes are deposited with fullerene (C_{70}) at different thicknesses of 10 nm, 50 nm and 100 nm by using thermal evaporation method. After deposition process, 100 nm thickness of silver electrode coated on the $Ti/Ti_2O/C_{70}$. To evaluate the shape, structure, and chemical compositions of the produced heterostructure, detailed characterizations were carried out. For the electrical properties of the $Ti/Ti_2O/C_{70}/Ag$ device, I-V and C-V measurements are performed under dry air condition from RT to 160 ^oC.

Keywords: TiO_2 nanotube, fullerene, anodization, heterostructure, electrical properties

References

[1] J. Lee, D. H. Kim, S.-H. Hong, and J. Y. Jho, doi: https://doi.org/10.1016/j.snb.2011.08.001.
[2] X. Chen and S. S. Mao, doi: 10.1021/cr0500535.
[3] S. K. Gharaei, M. Abbasnejad, and R. Maezono, doi: 10.1038/s41598-018-32130-w.
[4] P.-Y. Hsieh, Y.-H. Chiu, T.-H. Lai, M.-J. Fang, Y.-T. Wang, and Y.-J. Hsu, doi: 10.1021/acsami.8b17858.
[5] M. V. and S. G. Nebojša Zec, Nikola Cvjetićanin, Marija Bešter-Rogač, doi: 10.1149/2.0051708jes.
[6] R. F. C. and R. E. S. H.W. Kroto, J.R.Heath, S.C.O'Brien, Available: https://www.nature.com/articles/318162a0.

Microstructure and Magnetization Dynamics in $La_{2/3}Sr_{1/3}MnO_3$ Epitaxial Thin Films

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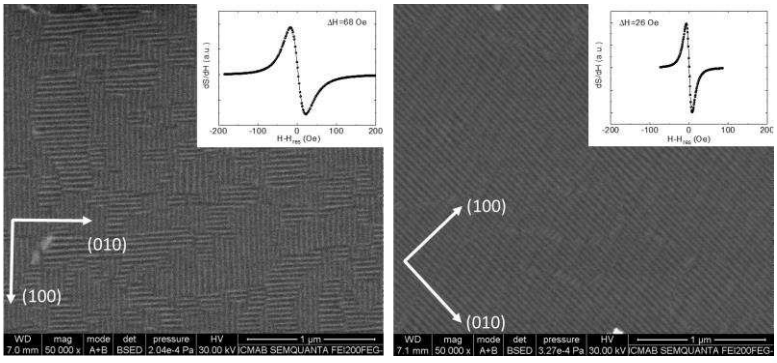
Keywords: Magnetization Dynamics, Ferromagnetic Resonance, Damping, Microstructure, Spintronic

Spintronics would allow access to electronic devices with lower power consumption and better performances than current semiconductor-based devices. The development of spintronics has boosted research aimed at optimizing and controlling the mechanisms for generating, manipulating and detecting spin currents, attracting intense attention to this field. On the other hand, in both generation (spin pumping is one of the most common methods) and transport of spin currents, magnetic dynamic properties of the materials are of major relevance. Magnetization dynamics is described through the Landau-Lifshitz-Gilbert Equation:

$$\partial \mathbf{M}(r,t)/\partial t = -\gamma \mathbf{M}(r,t) \times \mathbf{H}_{eff}(r,t) + (\alpha/Ms)\, \mathbf{M}(r,t) \times \partial \mathbf{M}(r,t)/\partial t$$

That includes the phenomenological Gilbert damping parameter, α, that is characteristic of each material and describes how magnetization relaxes. α, usually determined from the broadening of ferromagnetic resonance spectra, has both intrinsic and extrinsic contributions, the first are commonly related to spin-orbit coupling (SOC) while the second is usually related to the microstructural features of the material (inhomogeneities, magnetic impurities, grain boundaries, structural defects, structural strain, etc..). Owing to the inherent link between Gilbert damping and energy dissipation mechanisms, it has become one of the most important parameters for the development of energy efficient, low-consuming spin-based devices. In this work we present a study of the magnetization dynamics, by using ferromagnetic resonance (FMR) technique, in high quality $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) epitaxial thin film prepared by RF sputtering. Samples prepared by using off-axis and on-axis geometries have been studied. It is shown that even DC magnetic properties (saturation magnetization and Curie temperature) are identical, significant differences are found in their dynamic properties, with clearly distinct FMR spectra. Electron backscattered (EBS) images obtained in a field emission scanning electron microscope (SEM) revealed a close correlation between twins and FMR line broadening. LSMO samples having only one family of twin boundaries (single domain pattern) exhibit extremely narrow resonance lines while samples exhibiting the typical two domains twin boundaries pattern have broader resonance lines (see figure, where FMR measurements were taken at 300K and 8GHz).

In summary, this work demonstrates the great relevance of the microstructure in the magneto-dynamic performances of materials for their potential application in spintronics..



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Pulsed laser deposition of LaAlO3 films for MEMS applications

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Keywords: Pulsed Laser Deposition, microelectromechanical systems and freestanding thin films.

Different materials are emerging beyond silicon for the realization of microelectromechanical systems (MEMS) with enhanced functionalities. Oxide materials, and in particular epitaxial oxides, introduce new opportunities in terms of material properties and integration. Besides the current integration of oxides - such as PZT - with silicon, a full-oxides MEMS approach guarantees best material properties and fine tuning of epitaxy and strain. In this work, we study the growth of LaAlO3 (LAO) thin films on SrTiO3 (STO) substrates for the realization of freestanding thin film micrometric structures. LAO and STO are transparent materials in the visible range, so LAO/STO MEMS structures for optical devices can be envisaged. Furthermore, the micromachining process of STO substrates can be tailored by choosing their proper crystallographic cut [1].100 nm thin LAO films are grown by pulsed laser deposition and then patterned by optical lithography using ion milling and selective wet chemical etching. The mechanical properties of the LAO microresonators - such as their resonance frequency - are detected by a customized optomechanical setup.

We analyze the structural and morphological properties of the LAO films and their stoichiometry and make correlation with the growth, observing how the chosen parameters of the PLD process critically determine the amount of stress and the success of fabrication. The full epitaxy of the produced structures also allows the further growth by PLD of other functional epitaxial oxide layers directly on the prepared freestanding templates, thus enlarging the panorama of applications. This project has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement No. 828784 [2].

References:

[1] Plaza AE, Manca N, Bernini C, Marré D, Pellegrino L. The role of etching anisotropy in the fabrication of freestanding oxide microstructures on SrTiO3 (100), SrTiO3 (110), and SrTiO3 (111) substrates. Appl Phys Lett. 2021;119(3):033504. doi:10.1063/5.0056524

[2] www.oxinems.eu

Experimental and Theoretical Investigation of the Usability of Graphene-like 2D Crystals in Chemical Sensor Applications

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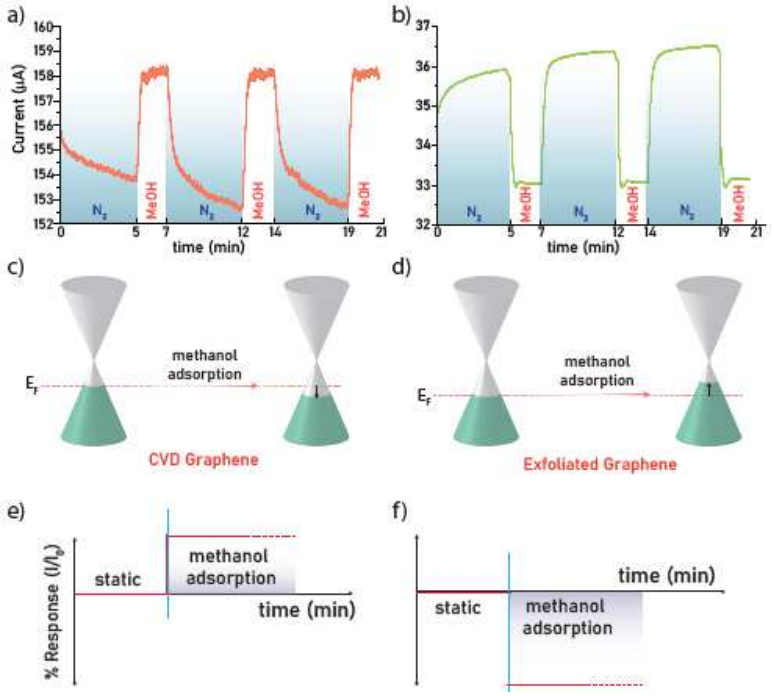
Keywords: Graphene, Functionalization, MoS2, Chemiresistor, Organic Compounds

The novel 2D materials such as graphene have already shown impressive VOC (volatile organic compound) gas monitoring performances as in sensitivity, limit of detection and response time. Herein, we draw attention to the inverse responses due to the different synthesis methods of graphene. While the graphene gas sensors fabricated by exfoliation decrease in current when exposed to methanol, CVD graphene gas sensors increase in current upon methanol introduction to the sensing surface. STEM images imply the population difference of edge sites, it is understood that while CVD graphene has very little amount of grain boundaries, exfoliated graphene is seen to be small sheets with high edge site population. Raman analysis indicate p-doping of both systems with a slightly more p-type character of exfoliated graphene. The charge transfer calculations indicate that carrier concentration is enhanced and diminished in CVD and exfoliated graphene, respectively. These results indicate that electrical nature of basal plane and edge sites of graphene affect the sensor response of the devices. Therefore, we carried out analyses of different sites of graphene and provided the theoretical and experimental findings to understand the reason of inverse responses of CVD and exfoliated graphene sensors at atomic scale.



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The Pimpinelli-Tonchev-Videcoq-Vladimirova (PTVV) theory: 21 years after

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The theory of bunching of straight steps on dynamic vicinal surfaces, the so called PimpinelliTonchev-Videcoq-Vladimirova (PTVV) theory, was published 21 years ago [1]. It is based on the Dimensional Analysis (DA) of a generic continuum equation for the time evolution of the surface slope during vicinal growth/sublimation to obtain observable exponents – these from the time-scalings of the bunch width and of the bunch size. The equation is built of two terms to account for opposite effects - the destabilizing role of the surface kinetics/diffusion asymmetry and the stabilizing role of the step-step repulsions. Later [2] the PTVV equation was modified to account for the existence of two limiting regimes – diffusion- and kinetics-limited ones. The numerical validation of the theory shows [3] that these effects are amplified by the correction for large surface slope. In the talk a complete numerical picture of the instability is drawn based on a detailed monitoring scheme [4] and careful DA [3,5]. It is compared with recent experimental results [6].

In collaboration with Magdalena Załuska-Kotur (Warsaw), Hristina Popova and Vassil Ivanov (Sofia) and Alberto Pimpinelli (Houston)

References

[1] A. Pimpinelli, V. Tonchev, A. Videcoq, and M. Vladimirova, Scaling and Universality of Self-Organized Patterns on Unstable Vicinal Surfaces, *Physical Review Letters* vol.88, 2061031 (2002).
[2] J. Krug, V. Tonchev, S. Stoyanov, and A. Pimpinelli, Scaling Properties of Step Bunches Induced by Sublimation and Related Mechanisms, *Physical Review B - Condensed Matter and Materials Physics* vol.71, 045412 (2005).
[3] F. Krzyżewski, M. Załuska-Kotur, A. Krasteva, H. Popova, and V. Tonchev, Scaling and Dynamic Stability of Model Vicinal Surfaces, Crystal Growth & Design vol.19, pp 821831 (2019).
[4] V. Tonchev, B. Ranguelov, H. Omi, and A. Pimpinelli, Scaling and Universality in Models of Step Bunching: The "C+–C-" Model, The European Physical Journal vol. B73, pp 539546 (2010).
[5] A. Krasteva, H. Popova, N. Akutsu, and V. Tonchev, Time Scaling Relations for Step Bunches from Models with Step-Step Attractions (B1-Type Models), in vol. 1722 (AIP Publishing, 2016), pp 220015.
[6] A. Kozlov, A. Samardak, N. Chernousov, H. Popova, M.A. Zaluska-Kotur, A. Pimpinelli, V. Tonchev, (2022). Predicted universality class of step bunching found on DC-heated Si (111) surfaces. arXiv preprint arXiv:2206.00190.

Growth mechanisms of 2D materials: the Kinetic Monte-Carlo point of view

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Keywords: 2D materials, kinetic Monte-Carlo simulations

Since the manipulation of graphene thanks to exfoliation, 2D materials have aroused an ever-growing interest as different materials form 2D layers (carbon, silicon, transition metal dichalcogenides …). They are expected to potentially surpass all previous technologies and their integration in devices has attracted great interest. Graphene is probably the most studied materials worldwide, due to its unique properties related to the Dirac-cone-shaped energy bands and high carrier mobility. However, despite significant efforts, there has been no reproducible method to open up its bandgap while preserving high carrier mobility. 2D Materials (2DM) based on group IV elements such as Si (silicene) and Ge (germanene) are promising alternatives.

The synthesis of silicene and germanene by epitaxy has been first reported on metallic substrates. However, their properties were found to be strongly affected by the coupling with their substrate and mixing effects between the substrate and the 2D film were revealed under certain conditions. In addition, fabrication of functional electronic devices necessarily requires non-metallic supports. One possibility is to introduce a buffer layer for decoupling the 2D adlayer from the substrate, as it has been recently proposed. Recent experiments concerning the epitaxial growth of Si on highly oriented pyrolytic graphite revealed the possibility to grow either 2D flakes with rather small sizes, or dewetted fractal islands. In any case, the understanding and control of the epitaxial growth of 2D materials is largely insufficient, and today's progress is limited by the lack of wafer-scale uniform growth that requires further investigation of dynamical mechanisms.

To progress in this direction, we developed kinetic Monte-Carlo (kMC) simulations of the epitaxy of silicene on various substrates, graphene and Ag(111). The challenge is to simulate out-of-equilibrium systems of sufficient size (typically of the order of a hundred nanometers) yet incorporating atomic details, over sufficiently long times (typically of the order of a minute or more) yet describing atomic events (diffusion, incorporation, exchange…). Accounting for appropriate effects, both dewetting and possible intermixing, we managed to rationalize new growth mechanisms specific of 2D growth. We reveal how intermixing can lead to a dramatic increase in island density at a transition where Si islands are inserted in a Ag substrate. We also revealed the possibility to grow large flakes of Si surrounded by a ridge for Si deposited on a Gr-6H-SiC substrate, in a given flux-temperature regime, as evidenced in experiments. We will discuss the new insights that may be drawn for the growth mechanisms of 2D systems.

Phase Stability of Thermoelectric ZnSb-SnTe Thin Films

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Keywords: thermoelectric materials, thin films, phase stability

Thermoelectric energy conversion has a number of advantages related to the compactness of devices, their high reliability, environmental friendliness, the possibility of use in a wide range of temperatures, etc. At the same time, the search for highly efficient thermoelectric (TE) materials, characterized by the maximum figure of merit ZT ($ZT=S^2\sigma T/\kappa$), recently, along with bulk semiconductor materials (Bi_2Te_3, Sb_2Te_3, PbTe, GeTe, etc.), mainly focused on the study of low-dimensional structures. This is due to the practical needs of collecting energy to power internet of things devices, utilizing waste heat from car exhaust gases, using body heat to power mobile devices and sensors, etc.

Unlike bulk samples, thin films have a number of advantages for TE devices, in particular, lower cost, lower mass, and the ability to synthesize on different substrates, which leads to miniaturization. At the same time, the advantages of microminiaturization have a reverse side, related to the difficulty of creating equal conditions for thin films growing, which often leads to their degradation and disintegration. Therefore, it is important to analyze the thermodynamic stability of multicomponent TE thin films along with the study of their kinetic parameters (electrical conductivity σ, thermal conductivity κ, and the Seebeck coefficient S).

High figure of merit values of the SnTe and ZnSb semiconductor compounds led to the idea of obtaining pseudo-binary alloys based on them. Recently synthesized $(ZnSb)_{1-x}(SnTe)_x$ thin films [1] showed an extremely high power factor ($PF = S^2\sigma$ = 3383 $\mu Wm^{-1}K^{-2}$ at 300°C for x = 0.273) due to the dielectric-metal transition as the result of SnSb nanoprecipitates formation. In the present paper, we have calculated the binodal and spinodal decomposition diagrams and critical decomposition temperatures of ZnSb-SnTe epitaxial thin films. Miscibility gaps were found using the lattice delta parameter model [2], taking into account both the deformation energy and the effects of plastic relaxation caused by mismatch dislocations. It is shown that, compared to the bulk samples, the studied films exhibit a narrowing of the spinodal decay interval and a decrease in the critical temperature. The critical thickness of pseudomorphic films was estimated depending on their composition and type of substrate. The occurrence of various types of biaxial deformations determines the distinctive nature of the compositional dependence of thin film's critical thickness. It was also shown that strain energy is the cause, from a thermodynamic point of view, of incoherent phase separation in the studied samples. Thus, the formation of SnSb nanoprecipitates is the main factor in the PF increase, which is consistent with the experimental data.

1. Wang, G., Zhang, Y., Lotnyk, A., Shi, H., & Chen, C. (2021). *Scripta Materialia*, 194, 113670.
2. Deibuk V. (2017). *J. Thermoelectricity*, No 1, 50-59.

Understanding Kinking of Semiconductor Nanowires

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Keywords: Semiconductor nanowires, vapor-liquid-solid growth, nucleation theory

Semiconductor nanowires are promising building blocks for a broad range of applications, including photovoltaics, solid state lighting, biosensing, as well as novel applications in quantum technology. Successful growth of nanowires can only be performed within a certain, materials specific parameter window, where the temperature at the growth interface and the reactant pressures are the most important parameters. Attempted nanowire growth outside of this window often lead to undesired growth features, such as tapering, kinking, or even ceased growth.

Kinking means a sudden change in nanowire growth direction. Several reasons for kinking have been reported. In heteroepitaxial nanowires, kinking at the heterointerface has been attributed to surface and interface energetic effects and been discussed in terms of the classical growth modes for heteroepitaxy [1]. In homoepitaxial nanowires, kinking can occur if the surface forces holding the particle at the nanowire tip are brought out of balance. Another reason is planar defects in the nanowire. Kinking can also be an effect of too low or too high reactant pressures or temperature. There is no conclusive understanding of why kinking occurs under these conditions. It has been suggested that at too low temperature the nanowire growth becomes unstable and at too high temperature the metal particle can be displaced [2].

In this investigation we focus on kinking in nanowires grown at too low temperature and too high reactant pressures. We propose that the reason for kinking at these conditions is related to an onset of 3D nucleation instead of 2D nucleation. First, we will introduce nucleation theory, and then we use nucleation modeling with realistic, thermodynamically assessed chemical potentials, to show that nanowire growth at certain conditions can lead to a situation where the supersaturation is high enough for 3D nucleation to be favourable over 2D nucleation. There is a high risk that 3D nucleation will lead to kinking while 2D nucleation is much more likely to result in straight nanowires. Our calculations indicate that the cross-over supersaturation for 2D-3D nucleation in gold catalyzed GaAs nanowires can be reached at easily attainable growth conditions. This means that kinking can indeed result from fluctuations or other sudden changes in growth parameters if the growth is carried out sufficiently close to this cross-over supersaturation. Finally, our modeling suggests promising routes for predictive control of kinking, which is of great benefit for advanced nanostructure design.

[1] K.A. Dick, S. Kodambaka, M.C. Reuter, K. Deppert, L. Samuelson, W. Seifert, L.R. Wallenberg, F.M. Ross, Nano Lett. 7 (2007) 1817-1822.
[2] S. Vlassov, S. Oras, B. Polyakov, E. Butanovs, A. Kyritsakis, V. Zadin, Cryst. Growth Des. 22 (2022) 871-892.

Wetting properties of heteroepitaxial systems determined from surface and interface energies calculations

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Keywords: Density Functional Theory, III-V/Si epitaxy, surface energy, interface energy, wetting.

Heterogeneous monolithic integration of dissimilar materials having different physical properties is today one of the most important challenges for epitaxy scientists. The clarification of wetting properties is one central issue during heterogeneous epitaxy, as it fundamentally governs the growth initiation and physical properties of the integrated materials and devices for photonics, electronics or energy harvesting applications. In this work, we use Density Functional Theory (DFT), with a fictitious hydrogen atoms charge compensation strategy, to determine the surface and interface absolute energies in the III-V/Si heterogeneous materials association case, analyze the wetting properties of IIIVs on Si,[1,2] and discuss the consequences [3,4]. We show that this methodology has been used effectively and could be extended to other heterogeneous materials. On the basis of DFT calculations, we finally demonstrate quantitatively that both the atomic/charge arrangement of the heterointerface (compensated or not),[5] and the nature of the first monoatomic layer at the substrate surface prior to the growth can dramatically affect the wetting properties.

This research was supported by the French National Research NUAGES Project (Grant no. ANR-21CE24-0006). DFT calculations were performed at FOTON Institute, and the work was granted access to the HPC resources of TGCC/CINES under the allocation A0120911434 made by GENCI.

[1] I. Lucci *et al.*, Physical Review Materials 2 (6), 060401 (R), (2018).
[2] I. Lucci *et al.*, Advanced Functional Materials, 28(30):1801585, (2018).
[3] C. Cornet *et al.*, Phys. Rev. Mater. 4, 053401 (2020).
[4] M. Rio Calvo *et al.*, Adv. Electron. Mater. 8, 2100777 (2022). [5] O. Supplie *et al.*, Phys. Rev. B 90, 235301 (2014).

Selective Area Growth of in-plane $In_{0.5}Ga_{0.5}P$ nanowires on $GaAs(111)_B$ substrate by molecular beam epitaxy

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Keywords : epitaxy ; nanowire ; InGaP ; atomic hydrogen ; selectivity

Selective area epitaxy of in-plane nanowire networks is a promising way to fabricate quantum devices with a scalable and reliable process [1]. However, this technique lacks of a method enabling the control of the charge density inside the semiconducting nanowire with a back-gate, as can be done with nanowires grown by VLS and subsequently transferred to a SiO_2 covered Si substrate. Among large bandgap semiconductors lattice matched to GaAs, $In_{0.5}Ga_{0.5}P$ received much attention as a promising alternative to $Al_{0.3}Ga_{0.7}As$ thanks to a larger direct bandgap ($\sim 1.9eV$), lower interface recombination velocity, less deep donor level, better wetting and oxidation resistance [2]. Growing selectively InGaP on a doped GaAs(111) substrate prior to the deposition of the low electron mass and strong spin-orbit coupling InGaAs, InAs or InSb channel could thus be a good option to offer an additional possibility of tuning the electron transport inside the quantum nanostructures. In this study, we show how atomic hydrogen assisted SA-MBE can be used to achieve in-plane InGaP nanowires and complex networks on $GaAs(111)_B$. The MBE system includes standard In and Ga effusion cells, a valved Arsenic cracker, a Phosphine high temperature injector and an atomic hydrogen RF plasma cell. Bare $GaAs(111)_B$ samples and SAG substrates, prepared with strip apertures of different sizes (down to 50 nm wide) and orientations inside a SiO_2 thin film deposited on $GaAs(111)_B$, are characterized *in-situ* by Reflexion High Energy Diffraction (RHEED) and *ex-situ* by Scanning Electron microscopy (SEM) and atomic force microscopy (AFM) respectively. Fig 1 and 2 display respectively SEM images of single NWs and AFM topography of NW networks after the deposition of a 50nm nominal thickness of InGaP at a growth rate of 0.2 ML/s and a temperature of 510°C. Under AFM, the NW topography is characterized with good accuracy, as the terraces coming from the layer-by-layer growth are visible. Further investigations about the electrical properties of the InGaP layer and the subsequent selective growth of InSb are now carried out and will be discussed during the conference.

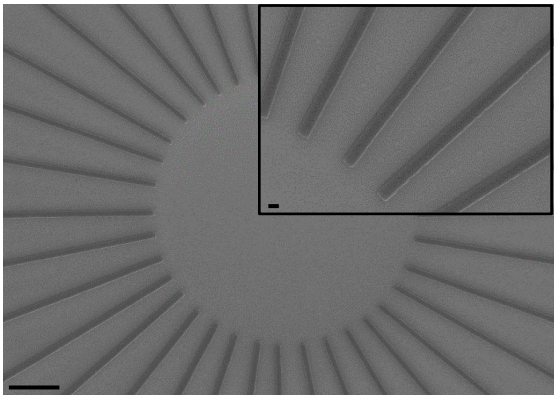

Figure 1: Plane-view SEM image of in-plane InGaP NWs grown inside 200nm wide mask apertures with an orientation variation every 10°. The vertical direction is along [0-11], the scale bar is 2µm and 200nm for the inset.

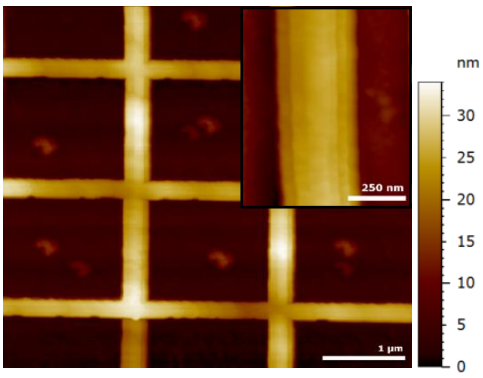

Figure 2: AFM image of a 200nm wide aperture NW grid pattern at 5µm scan size. Zoom on one of the NWs in the inset

References

[1] X. Yuan *et al.*, *Applied Physics Reviews*. 8, 021302 (2021)
[2] S. Xun-Zhong *et al.*, *Chinese Phys. Lett.* 20, 1616 (2003); N. Schmieder, p62. (2022).

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MBE growth of Si-based nanocrystal pyramids on pit-patterned Si(001)

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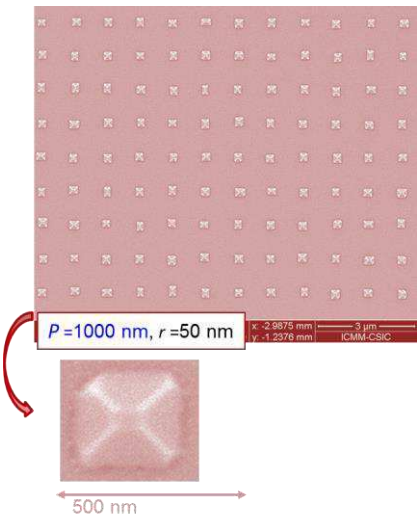
Keywords: nanocrystals; nanopatterning; lithography; epitaxy; self-assembly.

The controlled development of patterns at the nanoscale attracts great scientific and technological interest since it provides appropriate routes to achieve new surface and material functionalities with potential applications in a wide diversity of areas. The used methodologies often combine top-down and bottom-up strategies, in which any self-assembling phenomena of the synthesis procedure is promoted by a large scale pre-patterning of the substrate surface. By following this strategy we fabricate ordered arrays of Si-based nanocrystals with pyramidal shape, regular-size and controlled spatial arrangement. Such arrays could be interesting e.g. as templates for multi-dot configurations, in order to fabricate arrays of quantum-dots and quantum dot molecules of different materials.

We study the Molecular Beam Epitaxy (MBE) growth of this type of nanostructures on patterned areas ($25x25\mu m^2$) prepared by electron beam lithography (EBL) and reactive ion etching (RIE) on Si(001) wafers. Although similar strategies have been successfully used in Ge/Si(001), Ge/Si/Si(001) systems to produce highly regular arrays of Ge or GeSi islands and dots, for the Si/Si(001) system it was a challenge, since previous works only reported changes in the shape of the pre-pattern pits.

A variety of patterned fields are considered, formed by arrays of cylindrical pits with specific values of the nominal pattern periodicity (P), pit depth (d) and pit radius (r) in the ranges: 1500 nm ≤ P ≤ 370 nm; 100 ≤ r ≤ 35 nm; 80 ≤ d ≤ 27 nm. Thin Si layers (up to an equivalent layer thickness of 5 nm) are deposited by MBE on top of both flat and pit patterned Si(001) surfaces (previously exposed to HF vapor and annealed in UHV), using conditions in which the formation of nanoscale pyramid-like islands is promoted. Different values of substrate temperature and Si deposition rate are investigated, and our analysis focuses on two issues: i) island formation; ii) influence of the MBE growth conditions and geometry pattern parameters on the shape, size and spatial arrangement of the islands ("at" or "around" the patterned pits). A combination of chemical, morphological and crystal structure analysis techniques is used in the investigation: X-ray photoelectron and Auger electron spectroscopies, XPS, AES; atomic force and scanning electron microscopies, AFM, SEM; high and low energy electron diffraction, RHEED, LEED.



The SEM and AFM results show that, by choosing appropriate parameter sets of MBE growth conditions and lithography pattern features, the present methodology can be used to achieve a controlled positioning of the Si-based nanostructures, allowing also control of size, shape and number density of the pyramid-like nanocrystals (see Figure).

A position selective chemical analysis performed on these highly ordered nanopyramid arrays, by using XPS and AES (combined in situ with field emission SEM in a spectro-microscopy setup with micro/nano resolution, respectively), reveals significant details to understand and promote the formation of such nanopyramid crystals.

MBE-grown nanowires with wurtzite GaAs cores and ferromagnetic shells investigated by scanning transmission electron microscopy

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Keywords: core-shell nanowires, MBE, STEM, 4D-STEM

Hybrid nanostructures combining dissimilar materials are of high interest for novel technological solutions. Especially, semiconductor-ferromagnet nanowires (NWs) in the form of core-shell structures can provide a wide range of applications for spintronics as they allow to integrate common electronics with ferromagnetic materials and tailor new properties for future nanoscale devices. Development of such complex nanostructures became possible only after the progress in the synthesis, i.e. growing techniques such as molecular beam epitaxy (MBE) and characterization tools, i.e. transmission electron microscopy (TEM).

Here, we present NWs with semiconductor cores (based on wurtzite WZ-GaAs) and two types of ferromagnetic shells: 1) MnAs – soft ferromagnetic metal; 2) MnGa – hard ferromagnetic metal; all grown by MBE. We use TEM methods to characterize structural properties of the NWs: analysis of the interface between the core and the shell – their crystallographic orientation as well as the strain determination emerging in such systems due to the lattice mismatch. Figure 1 presents scanning TEM (STEM) images (panel a,b) obtained for type-1 NWs (with WZ-(Ga,In)As and MnAs shells) revealing their surface morphology, crystal structures (panel e) and diffraction patterns (panel c, d) obtained for the core and the shell allowing to reconstruct their interface and perform strain analysis.

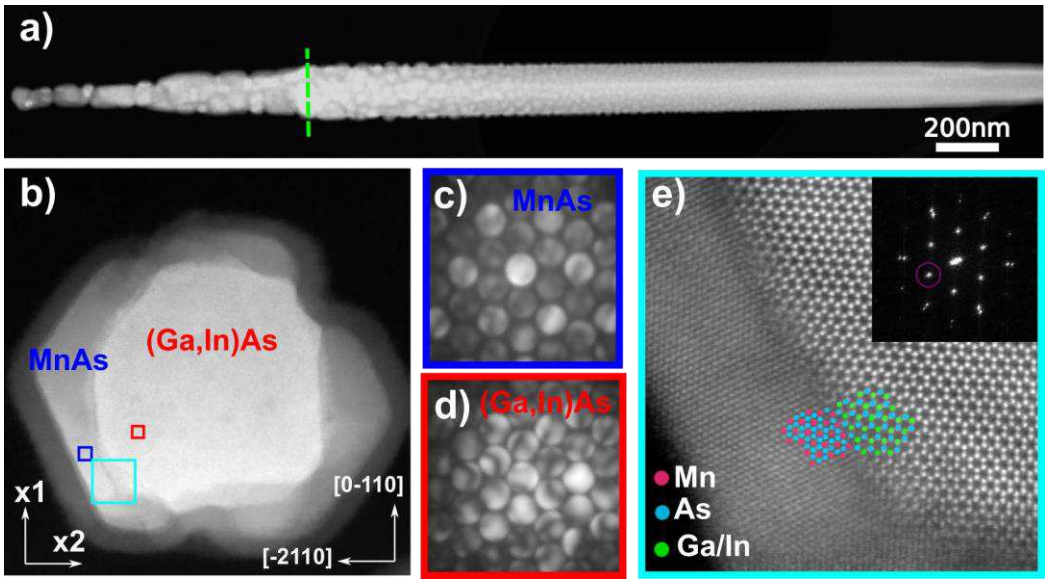

Figure 1 a) STEM image of the whole NW with its top on the left side of the image; green line indicates direction of the focused ion beam (FIB) cut made for NW cross-section, shown in b. b) STEM image of NW cross-section c) Nano-beam electron diffraction (NBED) from MnAs area highlighted in panel b with the dark blue box. d) NBED from (Ga,In)As area highlighted in panel b with the red box. e) High resolution (HR) STEM image of the light blue area in panel b containing (Ga,In)As and MnAs interface with crystal structures superimposed on the image; FFT of e is shown in the inset.

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Growth of few-layer van der Waals materials on semiconductor nanowires

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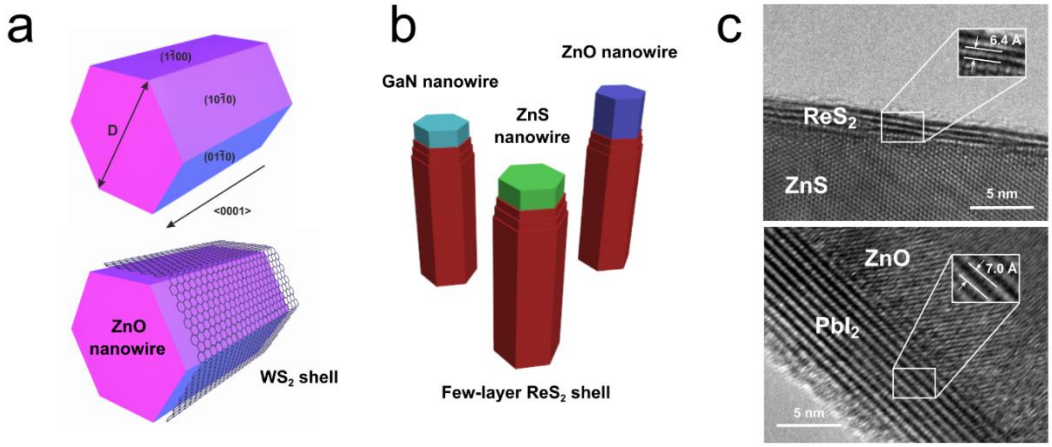
Keywords: nanowires; van der Waals materials; core-shell heterostructures; photodetection

Combination of different materials in complex nanowire (NW) heterostructures gives extra freedom to flexibly design their properties and add custom-made functionality, as well as NWs are a convenient template to study materials growth. First-time synthesis of various NW (e.g., ZnO, GaN) and layered van der Waals (vdW) material (e.g., WS_2 [1,2,3], MoS_2 [3] PbI_2 [4] ReS_2 [5]) core-shell heterostructures was demonstrated by combining different approaches, such as magnetron sputtering and chemical vapour deposition. Structural, compositional and optical characterization was performed. Single-NW photodetectors were fabricated to investigate the photoelectric properties of such hybrid materials. It was found that even a few-layer thin vdW material coating can significantly improve the photodetection properties of ZnO NWs by modifying the light absorption and spatial distribution of charge carriers. Such novel heterostructures could also be used for other applications in optoelectronics and in photo- or electrocatalytic hydrogen evolution reactions.

Fig. 1: (a,b) Schematic representation of different as-grown core-shell nanowires; (c) transmission



electron microscope images of different vdW material few-layer coating on nanowires.

[1] E. Butanovs, S. Vlassov, A. Kuzmin, S. Piskunov, J. Butikova, B. Polyakov. Fast-response single-nanowire photodetector based on ZnO/WS2 core/shell heterostructures. ACS Appl. Mater. Interfaces. 10, 13869-13876 (2018)
[2] B. Polyakov, K. Smits, A. Kuzmin, J. Zideluns, E. Butanovs, J. Butikova, S. Vlassov, S. Piskunov, Y. Zhukovskii. Unexpected epitaxial growth of a few WS2 layers on {11$\bar{2}$00} facets of ZnO nanowires. J. Phys. Chem. C. 120, 21451-21459 (2016)
[3] E. Butanovs, K. Kadiwala, A. Gopejenko, D. Bocharov, S. Piskunov, B. Polyakov. Different strategies for GaN-MoS2 and GaN-WS2 core–shell nanowire growth. Appl. Surf. Sci. 590, 153106 (2022)
[4] E. Butanovs, S. Piskunov, A. Zolotarjovs, B. Polyakov. Growth and characterization of PbI2-decorated ZnO nanowires for photodetection applications. J. Alloys Compd. 825, 154095 (2020)
[5] E. Butanovs et al. Synthesis and characterization of GaN/ReS2, ZnS/ReS2 and ZnO/ReS2 core/shell nanowire heterostructures. Appl. Surf. Sci. 536, 147841 (2021)

Growth and NMR study of high quality ordered $Mn_5(Si_x Ge_{1-x})_3$ thin films on Ge(111) substrate

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Keywords: Molecular beam epitaxy (MBE), Nuclear magnetic resonance (NMR), thin film, ferromagnetism, anti-ferromagnetism

In this presentation, the author will present the controlled and epitaxial growth of $Mn_5(Si_xGe_{1-x})_3$ thin films on Ge(111) substrate by Molecular beam epitaxy methods (co-deposition), as well as characterizations of their structural and magnetic properties by X-ray diffraction (XRD), Atomic force microscopy (AFM), Transmission electron microscopy (TEM), and Nuclear magnetic resonance (NMR).

Mn_5Ge_3 and Mn_5Si_3 are two compounds exhibiting hexagonal $D8_8$ structure (space group $P6_3/mcm$) and they can be grown epitaxially on Ge(111) substrates[1]. However, they exhibit very different magnetic behavior. Mn_5Ge_3 is a metallic ferromagnet that presents a high spin polarization of the conduction electrons at the Fermi level, a Curie temperature of 296K and a strong uniaxial magnetocrystalline anisotropy along the hexagonal c axis[2]. On the other hand, Mn_5Si_3 is an antiferromagnetic alloy exhibiting a (meta)magnetic phase transition: antiferromagnetic with a chiral spin structure below 65K and collinear above[3].

In earlier time, the electrical and magnetic properties of the bulk $Mn_5(Si_x Ge_{1-x})_3$ materials have only been studied in the bulk phase by few research groups[4,5]. Our work, studying on high quality ordered thin films, expands the structural and magnetic knowledge on these complex materials. ^{55}Mn NMR spectrum reveals the changes of local magnetic properties over Si concentrations. XRD shows the correlation between Si concentration and lattice structural parameter deformation and crystallinity. Through comprehensive analysis, we bring further insights on the transition between the ferromagnetic behaviors of the $Mn_5(Si_0 Ge_1)_3$ films and the anti-ferromagnetic $Mn_5(Si_1 Ge_0)_3$ films.

References

1. Zeng, C.; Erwin, S. C.; Feldman, L. C.; Li, A. P.; Jin, R.; Song, Y.; Thompson, J. R.; Weitering, H. H. Epitaxial Ferro magnetic Mn_5Ge_3 on Ge(111). *Appl. Phys. Lett.* **2003**, 83 (24), 5002 - 5004.

2. L Michez, A Spiesser, M Petit, S Bertaina, J-F Jacquot, D Dufeu, C Coudreau, M Jamet and V Le Thanh, Magnetic reversal in Mn_5Ge_3 thin films: an extensive study, J. Phys.: Condens. Matter 27 **2015** 266001

3. Sür gers, C.; Wolf, T.; Adelmann, P.; Kittler, W.; Fischer, G.; Löhneysen, H. Switching of a Large Anomalous Hall Effect between Metamagnetic Phases of a Non Collinear Antiferromagnet. *Nat. Publ. Gr.* **2017**, 1 - 7.

4. Panissod, P.; Qachaou, A.; Kappel, G. Inhomogeneous Transition from the Ferromagnetic State to the Antiferromagnetic State in $Mn_5(Ge_{1-x}Si_x)_3$ Alloys: an NMR Study. *J. Phys. C Solid State Phys.* **1984**, 17 (32), 5799 - 5810.

5. Zhao, F. Q.; Dagula, W.; Tegus, O.; Buschow, K. H. J. Magnetic Entropy Change in $Mn_5Ge_{3-x}Si_x$ Alloys. *J. Alloys Compd.* **2006**, 416 (1 2), 43 - 45.

Key parameters for GaP(111)$_B$ surface preparation and Selenium passivation

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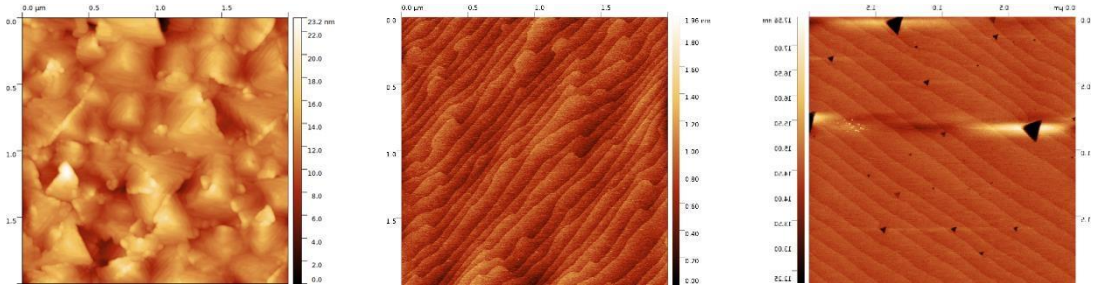
Keywords: III-V semiconductor epitaxy, GaP(111) surface morphology, Selenium passivation

GaAs(111)B has been shown to be a viable 3D substrate for the Van der Waals epitaxy of 2D-Transition Metal Dichalcogenides (TMDs) after a proper surface passivation treatment. Since rather high growth temperatures promote a better crystallographic quality of TMD layers, GaP might represent an interesting alternative to GaAs considering its higher thermal stability. However, the preparation of the GaP(111)B surface has been little reported in the literature with a resulting morphology revealing a rather high roughness without a well-defined long range order [1-3]. In this study, we present results relative to the preparation of well-ordered GaP(111)B surfaces and to their Selenium passivation. Substrates are deoxidized in a III-V MBE reactor under PH_3 and H_{at} fluxes to prepare clean GaP(111)B surfaces. Some of them are then transferred under UHV in a TMD epitaxial chamber and annealed under a Selenium flux with a Beam Equivalent Pressure in the 10^{-7}-10^{-5}T range. On other samples, a thin GaP buffer layer is grown before the Selenium treatment. Samples are characterized *in-situ* by Reflexion High Energy Diffraction (RHEED), X-Ray and UV photoemission spectroscopies (XPS/UPS) and *ex-situ* by Atomic Force Microscopy (AFM).

After deoxidization, the surface exhibits a 2x2 RHEED pattern and a morphology characterized by serrated steps whereas XPS does not revealed any residual contamination. Upon buffer layer growth, for temperatures below 650°C, the surface is rough with pyramidal shapes whose density increases when lowering the growth temperature. Above 650°C, a smoother morphology is obtained with regular steps, possibly with the formation of triangular holes at the highest temperatures. During Selenium passivation, the RHEED pattern shows a 1x1 reconstruction and whatever the temperature, it turns out that the Selenium flux should be kept near 10^{-7}T or below to avoid any significant subsurface component as revealed by XPS.



2 x 2 µm AFM images of a 60 nm thick GaP(111)B buffer layer grown at 540°C (left), 650°C (middle) and 670 °C (right)

[1] K. Hattori et al., Surface Science 525, pp. 57-65, 2003
[2] J.-B. Barakat et al., Journal of Crystal Growth 477, pp. 91-96, 2017 [3]
P. Kleinschmidt, Applied Surface Science 534, 147346, 2020

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Synchrotron based X-ray Absorption Fine Structure Spectroscopy and electronic structure calculations for materials

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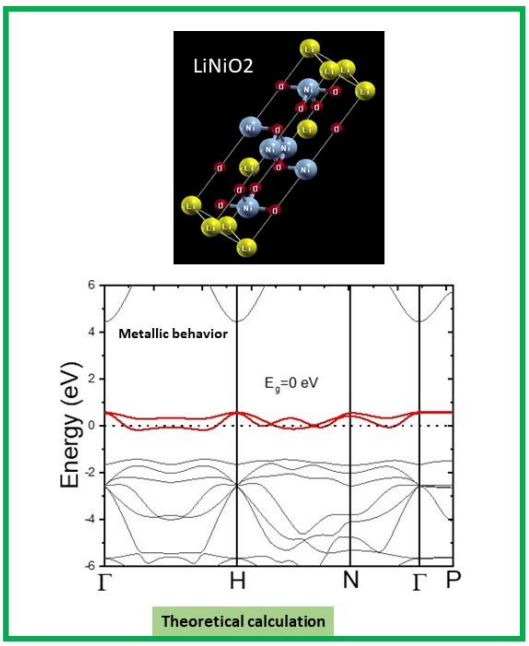
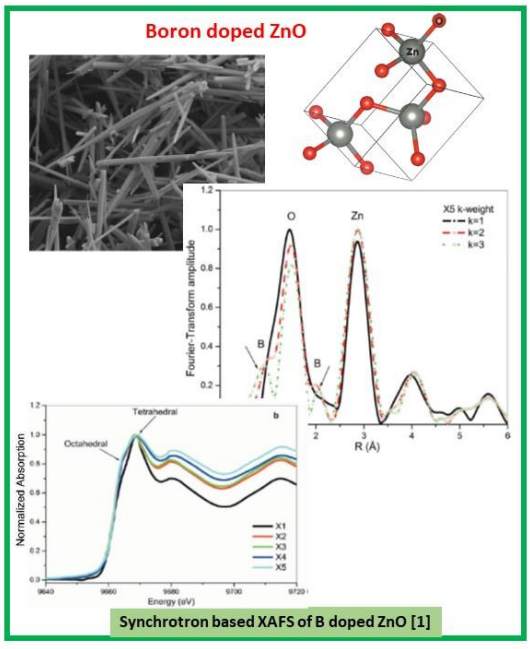
X-ray absorption fine structure (XAFS) spectroscopy is a useful technique to characterize both electronic structure and local structural properties of materials. XAFS can be considered in two parts: x-ray absorption near-edge structure (XANES) and extended x-ray absorption fine structure (EXAFS). Our group works on the correlation of crystallographic, electronic structure and transport properties of energy materials. The XAFS data of L-edge of Fe in LaFeO3 was measured and supported with Ligand Field Multiplet Calculation. At the SESAME synchrotron facility (Allan, Jordan), the XAFS data of boron doped ZnO were measured. Electronic and crystallographic structure analyses were carried out using the fitted spectra with the estimated spectra, by performing complementary k-weight analysis using the FEFF8.20 program. In theoretical part, computer simulation is strong tool to obtain the physical properties of compounds. Nowadays, there are several calculation program named "Wien2k, ABINIT, Vasp", etc. which are used to determine physical properties of compounds. The electronic structure of ZnO with and without dopant elements and recently LiNiO2 (LNO) battery material have been determined via Wien2k software depending on Density Functional Theory. For instance, the calculation density of state and electronic band structure of LNO with R-3m space group reveals that LNO has metallic characteristic which is in agreement with literature. More details about the experimental techniques and theoretical calculations from the point of the view of samples grown by epitaxial growth techniques will be presented along with the literature survey during the workshop. **Ref. 1:** Selma Erat et. al. J. Synchrotron Rad. (2021). 28, 448–454. **Keywords:** Electronic structure; Crystallographic structure; Synchrotron based XAFS; new materials; theoretical calculation.





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Impact of substrate doping on the performance of vertically illuminated Geon-Si photodetectors

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Keywords: LEPECVD, Heteroepitaxy, Ge-on-Si Photodiodes, Dark Current, Responsivity

Ge-on-Si photodiodes have been studied for more than twenty years, mainly for their application in integrated photonics in a waveguide configuration.
These devices tolerate fairly high dark current densities since the small volume and high optical power results in a sufficiently large signal to noise ratio.
Vertically illuminated photodetectors are instead required for imaging applications, of interest in the automotive and biomedical areas. In this case, a sufficiently low dark current density is required for the fabrication of multipixel devices.
Indium gallium arsenide is the state-of-the-art material for infrared imagers due to the lower dark current density ($\approx 10^{-7}$ A/cm^2) as compared to Ge-on-Si ($\approx 10^{-2}$ A/cm^2), but this kind of detectors are rather expensive (>10k€/device) while, Ge-on-Si photodetectors (~100€/device) can be produced in CMOS foundries.
The difference in the dark current of the two materials mainly arises from fundamental physical reasons. In fact, the dark current density is proportional to the intrinsic carrier concentration that is proportional to the effective masses. The direct band structure of the InGAs results in an electron effective mass ($m_e^*=0.037\ m_0$) substantially lower than that associated with L-valleys electrons in Ge ($m_e^*=0.22\ m_0$). As a consequence, for an indium gallium arsenide alloy featuring a 0.8 eV bandgap, *i.e.* equivalent to the direct-bandgap of germanium, the intrinsic carrier concentration is 50 times smaller than that of Ge.
Yet, the dark current of epitaxial Ge-on-Si devices is orders of magnitude larger than that of bulk Ge detectors, indicating that, despite the fundamental limits set by the Ge bandstructure, there's still room for reducing the reverse current of Ge epitaxial layers.
In recent years the reduction of threading dislocations and the implementation of surface passivation strategies have been investigated to reduce the dark current density. Instead, the effect of doping in the silicon-germanium heterostructure on the dark current has been not fully analysed.
To evaluate the impact of silicon substrate doping on dark current and photoresponse, a set of Ge-onSi photodiodes were grown by Low-Energy Plasma Enhanced Chemical Vapour Deposition **(LEPECVD)** and microfabricated by optical lithography and reactive ion etching.
All the investigated photodiodes feature a 1500 nm thick nominally intrinsic germanium layer, annealed to reduce the threading dislocation density, and heavily doped germanium top contact layer with a thickness of 100 nm. The silicon substrates doping has been varied from 10^{14} cm^{-3} to 10^{19} cm^{-3}.
Metal contacts are deposited by E-Beam Evaporator.
To characterize the photodiodes current/voltage measurements have been performed and clear trend between the dark current density and the doping levels of the substrates is observed.
Dark current in Ge-on-Si devices arises mainly from three mechanisms: diffusion, generationrecombination and trap-assisted tunneling. Temperature dependent I-V and C-V measurements have been performed to evaluate the relative weight of these three different mechanisms in determining the dark current. To characterize the photoresponse of the photodetectors, the responsivity has been measured in the wavelength range between 1300-1700 µm, for different reverse biases. Specific Detectivity has also been estimated as a figure of merit of the detector due to its dependence on both dark current and responsivity.

In-situ photoemission electron microscopy investigation of mono- and bilayer graphene growth on Ru $(10\bar{1}0)$

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Keywords: Growth, structure, substrate interaction

Epitaxial graphene growth has often been studied on close-packed transition metal substrates, e. g., the Ru(0001) surface, which is a well-studied model system for strong graphene-support interaction. Here, we focus on a Ru surface with different symmetry, i. e., the Ru $(10\bar{1}0)$ surface, to investigate the influence of the presumably modified graphene-substrate interaction on the growth of epitaxial monolayer and bilayer graphene (MLG, BLG) islands. The structural and chemical differences of the graphene on the two different surfaces are investigated by photoemission electron microscopy (PEEM), delivering information on both morphology and electronic structure. In-situ PEEM observation of graphene growth on the Ru $(10\bar{1}0)$ substrate by ethylene decomposition reveals the growth characteristics of MLG and BLG, the latter nucleating via surface segregation of carbon. In contrast to previous studies of the graphene/Ru(0001) system, graphene shows different growth characteristics depending on the growth temperature and relative orientation of the growing islands and surface steps seen in the figure below, whereas similar electronic properties seem to prevail. Yet, when the MLG is decoupled from the Ru $(10\bar{1}0)$ substrate via intercalation of oxygen, a distinct shift in work function is identified, slightly different from the respective shift on Ru(0001).

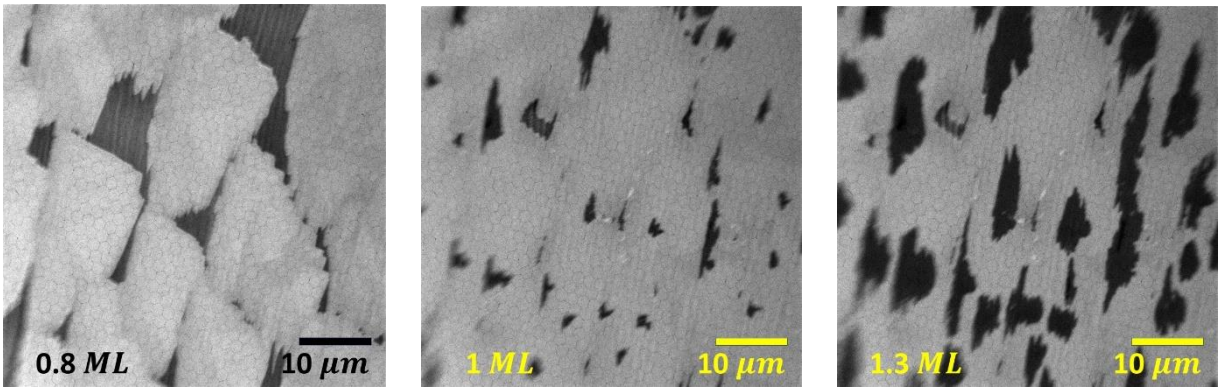

Figure 1: CVD prepared monolayer graphene growing second layer through surface segregation on Ru $(10\bar{1}0)$. The sample was prepared at 700°C and measured with photon energy of 4.9eV.

Growth of superconducting $YBa_2Cu_3O_{7-X}$ epitaxial layers by TLAG with in-situ synchroton characterization

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Keywords: TLAG, YBCO, epitaxy, superconducting materials, synchrotron X-rays

High Temperature Superconducting materials have very unique electrical and magnetic properties which makes them good candidates for applications in the energy sector, for ultrahigh magnetic field devices and transportation. However, their manufacturing costs are high due to the need of thick epitaxial films at km-length using thin film technologies. Therefore, low-cost chemical solution deposition (CSD) methods became very attractive for their fabrication. Among all CSD methods, we are working in the Transient Liquid Assisted Growth (TLAG), which is able to epitaxially grow thick $YBa_2Cu_3O_{7-X}$ (YBCO) films at even 2000 nm/s if the supersaturation conditions are properly controlled [1,2].

We use an environmentally friendly chemical process using metal-organic precursor solutions based on propionate salts giving us highly reproducible deposition and pyrolysis process that ensures a homogeneous nanocrystalline solid prior to the TLAG process [3]. Additionally, this method, let us use colloidal solutions with performed nanoparticles which can behave as pinning centers to improve the superconducting properties and obtain critical currents densities of 2.5 MA/cm^2 at 77K.

In this work, we have modified the molar composition (Ba/Cu) and rare earth ion (RE=Y, Gd) to change the supersaturation conditions during the transient liquid growth and facilitate the epitaxial growth. However, this growth process is done in non-equilibrium conditions, so kinetic parameters (like total pressure, heating ramps, pressure ramps or gas flow) are playing a relevant role. In order to study the influence of all these parameters, we have employed insitu XRD synchrotron experiments and determined the kinetic phase diagrams [2]. Synchrotron experiments were done at Soleil and ALBA, with a 2D detector acquiring images in the range of 100ms/image down to 9ms/image. We designed a system configuration built on a mobile rack coupling the XRD furnace with the gas and pressure systems. Additionally, it incorporates an in-situ mass spectrometer and an in-situ resistivity measurement. The information obtained from these experiments, together with the microstructure evaluation by advanced transmission electron microscopy, is being key to underpinning the TLAG-CSD growth mechanism and further improve the performances of the REBCO films.

[1] Soler, L., JAreño, J., Banchewski, J. et al. *Nat. Commun* **2020**, 11, 344.
[2] Rasi, S., Queraltó, A., Banchewski, J., et al. *Adv. Sci*. **2022**, 2203834.
[3] Saltarelli, L., Gupta, K., Rasi, S., et al. *Applied Materials & Interfaces* **2022,** *14* (43), 4858248597

Behavior of high-temperature-deposited CeO_x/Au(111) under reducing and oxidizing conditions

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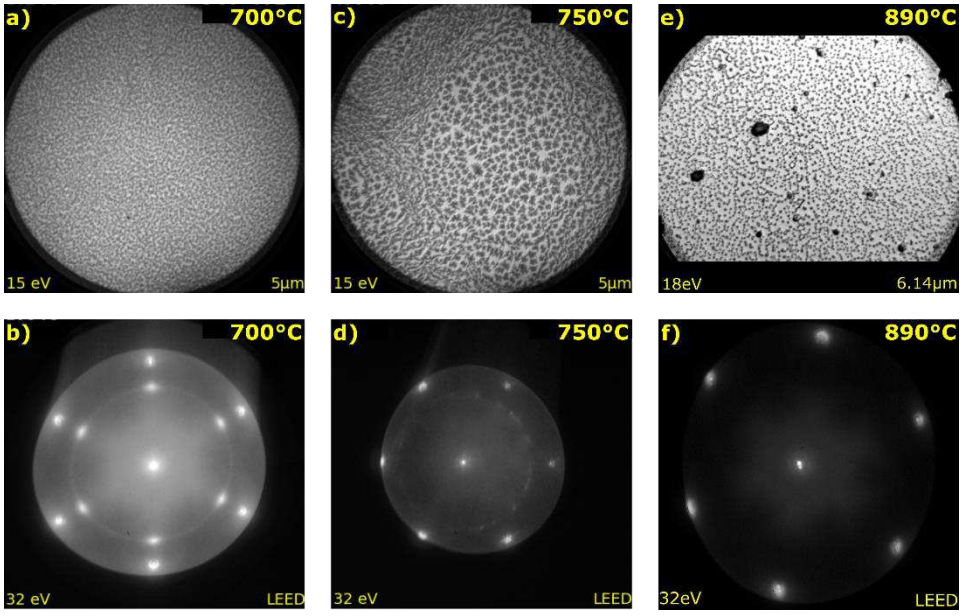
Keywords: Cerium Oxide, Au(111), Heterogeneous Catalysis

One of the most pressing challenges of modern catalysis is the development of new and improved catalysts to tackle a multitude of problems connected to the extensive use of fossil fuels and the resulting influence on global climate. In recent years, inverse metal-oxide catalysts consisting of oxide nanoparticles distributed on a metal support have received substantial research interest due to their beneficial properties such as high activity and selectivity compared to their conventional metal-oxide counterparts. This has been partly attributed to synergistic interactions between the metal and oxide constituents, so a detailed understanding of these effects is needed for rational and efficient catalyst design. In this study, we have explored the growth of cerium oxide nanoparticles on the Au(111) surface in situ and in real-time using low-energy electron microscopy (LEEM) and low-energy electron diffraction (LEED). An overview of the LEEM (a), c) & e)) and LEED (b), d) & f)) of CeO_x/Au(111) grown at different temperatures can be seen in the figure below. An explicit correlation between the deposition temperature and the structural properties of the oxide particles has been observed. Furthermore, the changes induced by the exposure to oxidizing and reducing gases under different conditions have been investigated. Comparing the behavior of cerium oxide nanoparticles grown on different substrates will allow first conclusions on the influence of the oxide-metal interaction on the structure and reactivity of the oxide nanoparticles.



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Experimental studies on PZT-LSMO heterostructures: mechanisms of ferroelectric stabilization and interface properties

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Keywords: Ferroelectrics, thin films, magnetoelectrics, heterostructures

Thin film heterostructures consisting of materials with ferroelectric and ferromagnetic properties are currently the focus of many research works due to their potential application in transducers, magnetoelectric sensors data storage & processing and energy harvesting devices.

Their interesting properties such as magnetoelectric (ME) coupling, tunneling electroresistance or tunnel magnetoresistance are coming from the interaction of orbital, lattice and spin degree of freedom. These are interfacial effects and are highly dependent on the structural quality of the films, chemical terminations of the subsequent layers and on the preparation conditions.

One example of FE/FM heterostructure is $Pb(Zr_{0.2}Ti_{0.8})O_3/La_{0.7}Sr_{0.3}MnO_3$ (PZT/LSMO) deposited on $SrTiO_3$(001). PZT and LSMO have several advantages that are: i) similar perovskite structure with small lattice misfit with each other and with the substrate, which allows preparation of high quality epitaxial structures with sharp interfaces; ii) PZT is ferroelectric with high polarization value in fully strained films grown on $SrTiO_3$(001) and iii) LSMO is half-metallic ferromagnet with nearly 100% spin-polarization.

In this work are presented results regarding the mechanism of ferroelectric stabilization for PZT/LSMO heterostructures obtained by pulsed laser deposition method on substrates with different work-functions and conduction type and the phenomena that appear at the interface between the PZT and LSMO films.

Unraveling the interface effects of atomic layer deposited ceria on metal oxide substrates

Carlos Morales[1*], Rudi Tschammer[1], Emilia Pożarowska[1], Yuliia Kosto[1], Malgorzata Kot[1], Carlos Alvarado[2], Christian Wenger[2], I. J. Villar-Garcia[3], V. Pérez-Dieste[3], K. Henkel[1], Jan Ingo Flege[1]

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Keywords: ceria, ALD, XPS, sensor, hydrogen

In the last decades, atomic layer deposition (ALD) has gained prominence in the materials and surface science communities owing to its high potential for integration as a scalable process in microelectronics. ALD's largest strengths are its well-controlled layer-by-layer deposition and growth conformity on 3D structures. Yet, the ALD technique is also well known to lead to amorphous and defective, non-stoichiometric thin films, resulting in modified materials properties that may even preferentially be used in certain applications. Interestingly, initial in situ X-ray photoemission spectroscopy (XPS) measurements of ceria ALD-deposits on Al_2O_3/Si, sapphire, and SiO_2 substrates confirm a Ce^{3+}/Ce^{4+} mixture dependent on the substrate interaction, deposit thickness, and morphology. Using near-ambient pressure XPS, we have significantly reduced ultrathin (< 10 nm) ceria films grown by ALD by exposing them to different O_2/H_2 partial pressures at moderate temperatures (< 525K). Notably, the total amount of reduction to Ce^{3+} is found to depend on the deposit thickness and initial ceria/substrate interaction. Furthermore, the intrinsic defects related to the ALD method seem to play a critical role in the reversible reduction at room temperature.

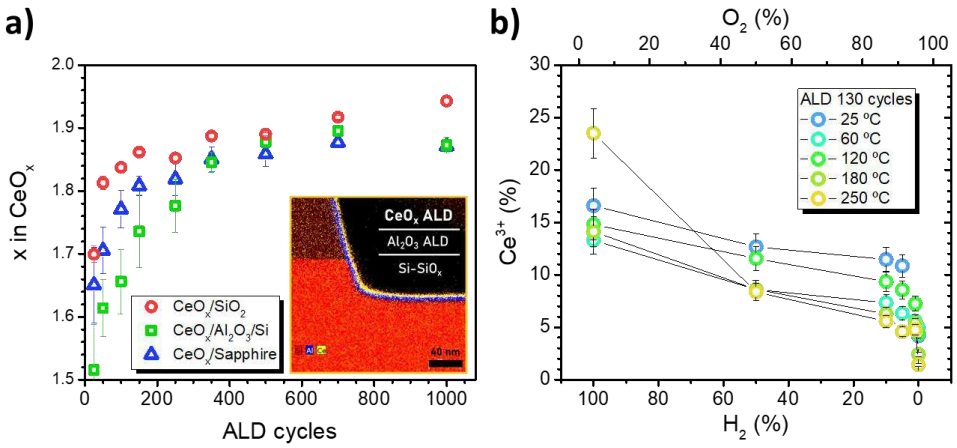

Figure a) Ce^{3+}/Ce^{4+} ratio as a function of the total number of ALD cycles and substrate; insert, transmission electron microscopy (TEM) cross-section image of the ALD-ceria ultrathin deposit. b) percentage of Ce^{3+} states as a function of H_2/O_2 mixture for different sample temperatures.

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Development and characterization of epitaxial metal oxide layers for resistive random-access memory

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Keywords: Epitaxial thin films, Functional oxides, Resistive switching

Transition metal oxides, such as Y_2O_3, TiO_2, HfO_2, MoO_3, have many unique properties, what makes them excellent candidates for use in the electronics industries. Under electrical stimulation their resistance can be changed. This phenomenon is called resistive switching and is used in the ReRAM memory (resistive random-access memory). Memory of this type is most often in the form of a MIM (metal-insulator-metal) layered structure. Electrical stimulation causes the formation of conductive filaments in the insulator layer, which leads to changes of its state. Resistance can be changed between high resistive state (HRS) and low resistive state (LRS). Gradual transition between these two states enables the stabilization of intermediate resistance levels, a quality that makes ReRAM attractive for multi-state memory and artificial synapse applications.

The research based on the stabilization of intermediate resistive states in oxygen-engineered yttrium oxide-based resistive switching devices will be presented. The analysis was performed on MIM structures with epitaxially grown yttrium oxide used as the functional layer, with titanium nitride bottom and platinum top electrode [1-3]. Yttria layers were deposited by the e-beam evaporation method in UHV conditions with different oxygen radical flows during the growth process. These conditions allow to achieve various stoichiometry and phases in transition metal oxides that have impact on the electrical characteristics and device performance. Investigations confirmed that samples produced with low oxygen flow are forming-free, requiring low voltages to create the filament, while with increasing oxidation conditions, the forming voltage increases [1]. In the reset process, the gradual switching transitioned to more abrupt characteristics with increasing degree of oxidation. Multilevel resistive switching studies showed that the number of intermediate states stabilized by varying the voltage applied during reset strongly depend on the oxidation conditions used in the growth process. Samples with the lowest oxygen concentration have the highest number of intermediate states, which decreases with increasing oxygen content. In all investigated stoichiometries a high stability of the resistive states was observed.

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[1] S. Petzold, E. Piros *et al.*, *Tailoring the switching dynamics in yttrium oxide-based RRAM devices by oxygen engineering: From digital to multi-level quantization toward analog switching,* Adv. Electron. Mater. **6**, 2000439 (2020)
[2] E. Piros et al., *Role of oxygen defects in conductive-filament formation in Y_2O_3-based analog RRAM devices as revealed by fluctuation spectroscopy,* Phys. Rev. Applied **14**, 034029 (2020)
[3] E. Piros et al., *Enhanced thermal stability of yttrium oxide-based RRAM devices with inhomogeneous Schottky-barrier***,** Appl. Phys. Lett. **117**, 013504 (2020)

Numerical and experimental study of the effects of the carrier gas in MOCVD growth

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Keywords: Numerical simulation, carrier gas, MOCVD, epitaxial growth, hydrodynamics.

Abstract: The carrier gas plays a key role during growth by MOCVD since it dramatically determines the hydrodynamic and thermodynamic conditions in the reactor, which affect the physical and structural properties of the grown crystal. However, the effects of the carrier gas in the growth can be difficult to characterize in a closed system like an MOCVD reactor.

In order to understand the implications of using a specific carrier gas, a two-step study has been developed. For this, we combine the results of numerical simulations performed with the software COMSOL Multiphysics with sets of growths whose results can be correlated with the main features shown by the simulations.

In this presentation, we will show the implications of the carrier gas election regarding the hydrodynamic conditions, temperature gradient and precursor mixing. The simulations, which have been programmed to describe our equipment, a horizontal two-inlet MOCVD reactor (*Quantax 226*), have been carried out for both light gases, such as H_2 and He and heavier gases, like N_2 and Ar. Moreover, these simulations will be correlated with a series of growths of CdO and the ternary alloy CdZnO with different morphologies (thin films and nanoparticles) on r-sapphire and GaAs substrates, performed with N_2 and He. We will show that key features of the crystal properties like morphology or composition are greatly affected by the carrier gas choice.

Hexagonal Boron Nitride: epitaxial growth and wet transfer tuning

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Keywords: hBN, epitaxy, wet chemical transfer, graphene, Raman Spectroscopy

In the last decade, there has been a significant interest increase in layered two-dimensional (2D) materials with graphene as the first representative of the entire family. Soon after the discovery of graphene, it turned out that more complicated compounds could take the form of 2D crystals. It has also been shown that it is possible to build non-natural hybrid materials by stacking layers of different 2D materials. This opened new perspectives in the application of such different types of hybrids in electronics, optoelectronics[1] and spintronics.

The group of 2D materials includes hexagonal boron nitride (hBN), which, is one of the most important van der Waals materials.[2] It has a honeycomb structure similar to graphene but is insulator with a high dielectric constant.[3] In addition, thin layers of hBN are transparent and mechanically and chemically stable, so they can be used to build a new type of transparent and flexible electronic devices.[4–6] Several examples of the multilayer and polycrystalline hBN synthesis by means of chemical vapor deposition (CVD) have already been described in the literature.[7]

The only ultra-pure hBN single crystal on the market today is the material produced under extreme pressure[8] which is characterized by very small lateral dimensions. This implies many difficulties with handling and potential application of hBN in electronic industry beyond proof-of-concept devices. In practice centimeters sized crystals[9] are required to use hBN as an encapsulation layer or as barrier substrates for 2D semiconductors. Unfortunately, obtaining macroscopically sized monolayer hBN crystals remains a major challenge.[7]

The only known way to get hBN as a large-area monolayers with low amount of defects is grown by molecular beam epitaxy (MBE). Recent experiments show that this is possible.

During the STSM, I focused on the transfer of graphene from a copper substrate to silicon and I took part in the growth of hexagonal boron nitride by means of molecular beam epitaxy as well as wet chemical transfer of this material from nickel to other substrates. During the STSM, I participated in the development of a technology for cleaning graphene and hBN surfaces from contamination.

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[1]Shi, Z. *et al. Nature Communications* **11**, 1–8 (2020)
[2]Yankowitz, M., *et al. Nature Reviews Physics* **1**, 112–125 (2019)
[3]Lu, S. *et al. Nature Communications* **13**, 1–10 (2022)
[4]Choi, S. H. & Kim, S. M. *Nature* **606**, 37–38 (2022)
[5]Ciarrocchi, A., *et al. Nature Reviews Materials* **7**, 449–464 (2022)
[6]Haastrup, S. *et al. 2d Mater* **5**, 042002 (2018)
[7]Uchida, Y. *et al. ACS Nano* **12**, 6236–6244 (2018)
[8]Taniguchi, T. & Watanabe, K. *J Cryst Growth* **303**, 525–529 (2007).
[9]Dong, J., *et al. Nature Communications* **11**, 1–8 (2020).

Transmission electron microscopy of Hybrid Heussler alloy-based structures

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Keywords: Heussler Alloy, Transmission Electron Microscopy, Structural analysis

The detection of magnetic fields with increased spatial resolution to micro-nanoscales is very important for magnetometry [1]. It is of great interest to have low-dimension sensors with increased sensitivity and extended capabilities. The discovery of magnetoresistive (MR) effects (AMR, TMR, GMR and CMR) in magnetic structures encouraged fundamental research leading to a number of laboratory-scale and commercially available devices [2]. Moreover, nowadays, the magnetosensorics becomes very important for wearable electronics and soft robotics. Each application has its specific requirements for sensitivity, temperature and magnetic field ranges of operation, accuracy, sensor's positioning, etc. Therefore, the choice of material with specific properties and design of sensing element becomes very important.

High-resolution transmission electron microscopy (HRTEM) study on layered Heusler alloy Co_2MnSi structures is presented in this work. These films were grown by using magnetron sputtering, serves as a main active element of magnetoresistive sensor with tunable sensitivity. Series of samples, including dependence on layers' thicknesses (5 - 200 nm) and annealing temperature (400-650 ^{o}C) were analysed. Such novel hybrid sensor would provide possibilities to decrease its dimensions for measuring magnetic fields in small volumes, especially for measurement of field direction in respect to reference plane, when in conventional methods three sensors are used. Other complex structures, including LSMO based sensors, were also analysed.

High-resolution TEM image (Fig. 1) show multi layered structure of FeNi-Cu-FeNi Heussler alloy structure. Individual layer thicknesses and structure was determined.

These structural peculiarities, unresolvable by other techniques, affect magnetic properties, such as magnetoresistance anisotropy and sensor sensitivity, so in-depth structural analysis is crucial in sensor development and could be used for the development of magnetic field sensors with predetermined parameters for operation at low or high temperatures.

This project has received funding from the Research Council of Lithuania (LMTLT), agreement No. S-PD-22-6

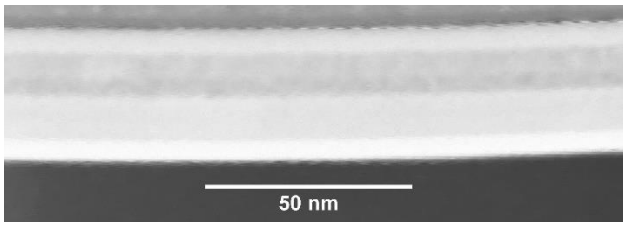

Fig. 1. High-resolution STEM image of a multilayer Heussler alloy structure

References

[1] Pisana et al. Nano Lett. 2010, 10, 341, DOI:10.1021/nl903690y
[2] Zheng et al, IEEE Trans. Magn. 2019, 55, 0800130, DOI: 10.1109/TMAG.2019.2896036

Epitaxial growth of MoS_2 on sapphire and mica

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Keywords: MoS_2, TMDC, epitaxial growth, CVD

TMDCs (Transition Metal Dichalcogenides) attract tremendous interest because of their intriguing properties such as large band gap, high current on/off ratio at room temperature, spin-valley polarization, large spin-orbit splitting, valley Hall effect, superconductivity and anomalous giant magnetoresistance [1]. This makes high-quality TMDCs necessary in practical applications. CVD (Chemical Vapor Deposition) is an effective method to grow large area TMDCs films.
Here, we report on the epitaxial growth of highly-aligned molybdenum disulfide (MoS_2) on c-plane sapphire and mica by chemical vapor deposition (CVD). The obtained MoS_2 was studied by XRD, Raman spectroscopy, TEM and XPS. It is found that the he ratio of sulfur and molybdenum trioxide (MoO_3) precursor, reaction temperatures and gas flow plays an essential role in the epitaxial CVD process.

Reference:
[1] Seoung-Woong Park et. al., Synthesis of Large-Scale Transition Metal Di-chalcogenides for Their Commercialization. Applied Science and Convergence Technology 2020; 29(6): 133-142

Acknowledgement: We are grateful to the financial support of COST Action CA20116 OPERA « European Network for Innovative and Advanced Epitaxy » and Bulgarian Science Fund under the project numbers FNI COST/15 and FNI КП-06-ДО 02/2 in the frames of M-ERA program project "Functional 2D materials and heterostructures for hybrid spintronic-memristive devices"

Polarization stability and interface termination dependence in ferroelectric heterostructures

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Keywords: polarization, dft, heterostructures, stability

Ferroelectric polarization in materials such as $PbTiO_3$(PTO) and its more popular brother $Pb(Zr_xTi_{1-x})O_3$ has been the subject of extensive numerical studies for both bulk and to some extent multilayered structure systems. Recent experimental investigations have revealed that if a condenser-like metal-ferroelectric-metal (MFM) structure is modified to include a thin film insulating layer at one of the interfaces, the electric properties of the device changes significantly. This may lead to new types of applications for these types of structures, such as energy storage and multi-bit memories.
In this study we have used density functional theory (DFT) methods implemented in Quantum Espresso to investigate the stability of ferroelectric polarization in MFM and MFIM structures (where an insulator was added between the ferroelectric and the metal electrode) for different interface terminations of the ferroelectric layer.
The most common materials used in experiments to fabricate such devices are $SrRuO_3$ which has a metallic conduction and is usually used as an electrode and $SrTiO_3$ which is an insulator.
For all calculations, a slab configuration was used with a 20 Å vacuum region surrounding the device on both sides. Previous numerical studies, have shown that a ferroelectric layer in a multilayer structure must have a thickness of at least 7 unit cells in order to exhibit two stable polarization states. In order to keep the structure small, the SRO electrodes were 3 unit cells each and the same was chosen for the STO layer. Total energy relative to the energy of the centrosimetric state versus ferroelectric distortion curves have been obtained (see below) for different terminations of the ferroelectric layer for the MFM and MFIM structures. The results show a strong influence of the insulator layer on the preferred polarization orientation of the ferroelectric layer. The interface termination also plays an important role in determining the magnitude and stability of polarization in the ferroelectric layer.

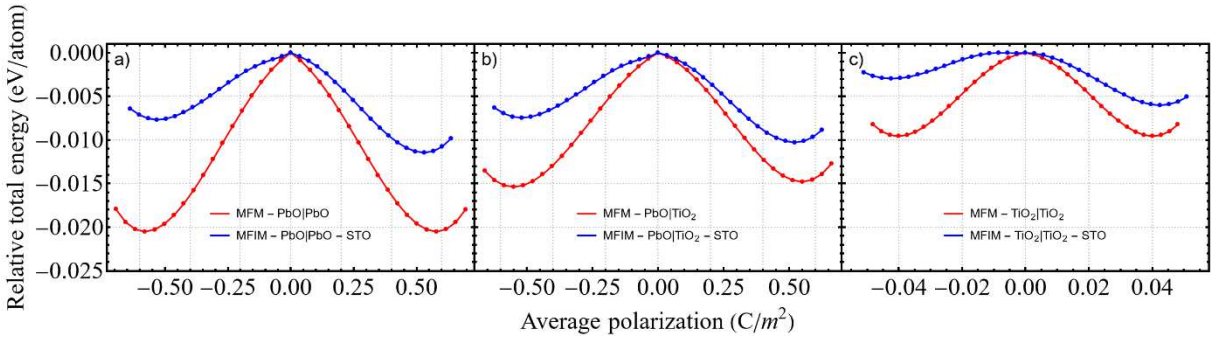

Figure 1 : Relative total energy as a function of the ferroelectric distortion for three terminations of the ferroelectric layer: a) begins and ends with PbO layer; b) begins with PbO and ends in a TiO_2 layer and c) begins and ends with a TiO_2 layer. Red curves are for the MFM structure, while the blue is for MFIM.

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Synthesis of microgels by microfluidics

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Keywords: soft colloidal lithography, microgels, microfluidics, self-assembly

Soft colloidal lithography is a low-cost and scalable technique which relies in the self-assembly of microgels at fluid interfaces to form ordered monolayers which can be transferred to solid substrates. These microgels can carry inorganic cores such as gold nanoparticles, which can act as seeds for epitaxy. Once the monolayer is deposited, the polymer can be removed via plasma ashing, obtaining self-assembled arrays of inorganic nanoparticles with complex orderings [1]. The compression of the soft microgels at the interface at varying surface pressures allows fine tuning of the core-to-core distance of the array. Nevertheless, the maximum separation is given by the size of the microgels, and current synthesis routes such as precipitation polymerization produce microgels with diameters up to ~1 µm. Thus, to increase the spacing between the features of the array it is necessary to explore new synthesis routes which allow the fabrication of bigger microgels. In this STSM, the grantee visited the Centre de la Recherche Paul Pascal for 2 months to design and fabricate microfluidic devices aimed to synthesize microgels up to 100 µm. A pre-gel solution containing the monomer, crosslinker and UV initiator was injected together with mineral oil inside the microfluidic device to produce monodisperse microdrops of tunable size which could be polymerized via UV-irradiation (Fig. 1a). We designed the masters and replicated them in PDMS, focusing on transferring the technique to the University of Granada. A balance between size control and UV time exposure to produce the polymerization can be achieved by controlling the flow rates of both phases. Finally, as reported in Figure 1b, the technique was successfully transferred to the University of Granada.

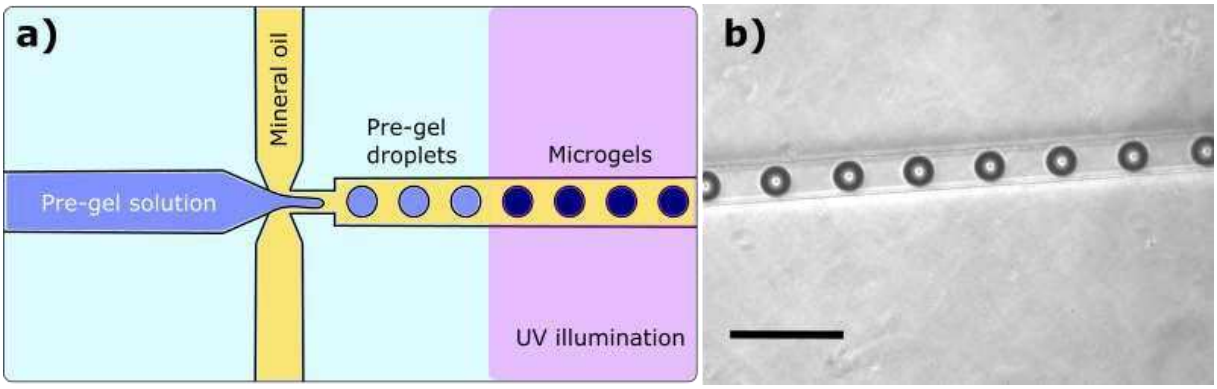

Figure 1. a) Schematic of the microfluidic device fabricated for the microgel synthesis. b) Microdrops obtained in the University of Granada after transferring the technique. Scale bar: 500 µm.

[1] Fernandez-Rodriguez et al. Tunable 2D binary colloidal alloys for soft nanotemplating. *Nanoscale*, 2018, 10(47):22189-22195.

Characterization of ferroelectric multilayered structures based on doped PZT thin films

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Keywords: ferroelectric, epitaxy, doping, electric properties, new applications.

Alternation of several different layers of ferroelectric materials or the joining of a ferroelectric and an insulator determines different interactions and electrostatic couplings. The resulting electrical characteristics are different from those of the constituent materials and can be used for new applications in electronics.
For this study, structures such as PZT(Fe)/PZT(Bi), PZT(Fe)/PZT(Nb) or PZT(Fe)/STO/PZT(Bi) were analyzed. These multilayered structures consist of successive thin films obtained by pulsed laser deposition (PLD) on a SrTiO3 (STO) substrate covered with a thin layer of SrRuO3 (SRO) as bottom electrode. Structural characterization performed by XRD and TEM proves the epitaxial growth of the structures.
Fe and Bi doping of PZT has the role of changing the conduction type as is the case with semiconductors. Fe and Nb elements are B-site doping type in the perovskite structure of PZT and have the role of increasing the hole charge density and electron charge density, respectively. On the other hand, doping with Bi element is an A-site doping type and giving an increased electron density. Beside changing conductivity type, many other electric characteristics (eg polarization, coercive voltage, dielectric constant) are changed by dopants.
The construction of multilayered structures using thin films of doped PZT determines different structural and electric properties that strongly depend on the choice of the constituent layers, the presence of an insulator interlayer but also on the deposition sequence.
New potential applications could be developed based on the special electric characteristics of the multilayered structures such as: multi-bit memories, non-destructive reading memories, super capacitors for energy storage or neuromorphic computing.

Germanium Quantum Wells for Spin Qubit Applications

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Keywords: qubits, LEPECVD, heteroepitaxy, germanium quantum wells

Over the past few years, interest in quantum computing has increased exponentially, with the spin degree of freedom of electrons or holes in semiconductor quantum dots (QDs) representing one (among many) possible qubit realization schemes. Hole spin qubits are created by electrostatically gating a 2DHG to define QDs with discrete energy levels, and the spin states are Zeeman-split by a magnetic field.

Germanium is the mainstream semiconductor with the highest p-type mobility, a feature leading to a renewed interest for Ge applications beyond the dominance of silicon. Ge quantum wells (QWs), are attracting interest due to possible applications which benefit not only from the properties of the 2dimensional hole gas (2DHG) formed in the QW, but also from the compatibility of SiGe with Si-based growth and fabrication.

The epitaxial growth of the Ge QW, cladded by barriers with relatively high Ge content, can be achieved following two different approaches: a reverse graded buffer, in which, starting from pure germanium, the Si content is increased up to the final amount, or a forward graded buffer, where starting from pure silicon the Ge concentration is linearly increased.

Material quality is a critical factor for qubit performances. The characterization of the electrical properties of the 2DHG by Hall measurements at cryogenic temperatures is a typical and effective approach.

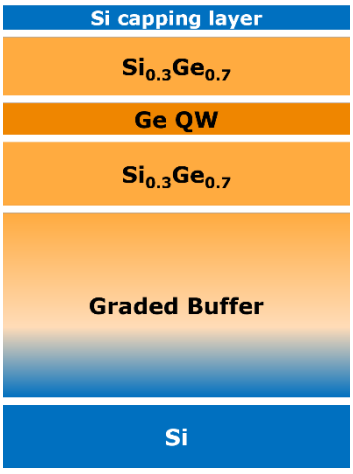

Figure 1 Schematic view of the grown structure

A Ge QW has been grown by a plasma-activated variant of chemical vapor deposition, LEPECVD (low-energy plasma-enhanced CVD) on a $Si_{0.3}Ge_{0.7}$ substrate on top of a virtual substrate. LEPECVD is a fast and efficient growth technique, so a relatively thick (several microns) forward graded buffer with a linearly graded concentration profile from pure Si to $Si_{0.3}Ge_{0.7}$ can be used as a buffer layer (Figure 1).

The growth rate can also be decoupled respect to the substrate temperature. This allowed a reduction of substrate temperature, helping to mitigate interdiffusion effects and strain-induced roughening at the QW interfaces. The sample has been then structurally characterized by HR-XRD.

Electrical characterization measurements were performed at low temperature (1.6-10 K) on Hall bar devices, resulting in a mobility exceeding 100000 cm^2/Vs. A scattering mechanisms analysis has been performed, highlighting the impact on mobility and dingle ratio of each considered mechanism. The percolation density, one of the most relevant figures of merit for qubit stability, has been extracted, with a value of around 10^{11} cm^{-2}.

Shubnikov–de Haas (SdH) oscillations and quantum Hall effect were observed, allowing the extraction of the Landau level lifetime, that proved to be high compared to the momentum lifetime, which may help to explain the excellent results obtained by collaborating research groups which fabricated qubits on this material.

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Electric-field engineered lattice distortions for optoelectronic devices

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Keywords: strain-engineering, orbital-ordering, optoelectronics

In strongly correlated materials the physical properties are inherently associated electronic degrees of freedom, yielding the possibility to control them by an applied electric-field (E-field). Although magnetic properties can already be controlled by an E-field at room-temperature, it is not yet the case for electronic, structural, and optic properties. This control is most effective in materials that present a metal-insulator transitions (MIT) mediated orbital ordering (OO) phenomena that can be found among $RNiO_3$, $AFeO_3$ and $RMnO_3$ compounds, whose B-site *d*-orbitals are characterized by e_g^1 occupation [1,2]. The aim of this work is to strain-engineer strongly correlated perovskites to achieve an unprecedent E-field control of electronic transport and optic properties, where the key driving forces are ultimately grounded on their distinctive cross-coupling between different degrees of freedom.

It is currently rare to find materials wherein E-field tuning of their physical properties is efficient enough to fulfil the high-standards required for applications. To provide E-field tunable functionalities in a single optoelectronic device is a major unprecedentedly reported step. So far, the pursued methodologies were to assembly multiple devices with different fabrication parameters (e.g. microstructuring, defect concentration) in order to vary their working specifications. We are implementing a new route, based on recent theoretically predictions regarding specific strain-engineering in strongly correlated perovskites, that can enable the E-field control of their OO, associated structural distortions and physical properties, such as MIT [1-2]. Our proposed course is noteworthy for a number of optoelectronic applications, such as solar cells with E-field controllable photocurrent direction, remote infra-red radiation detection, light-controlled memresistive memories, tip-enhanced photovoltaic effect, and negative charge transfer effect.

This work addresses OO, intimately linked to electronic degrees of freedom that also drive other structural (e.g. Jahn-Teller distortion), optic (e.g. bandgap) and magnetic properties. OO is intrinsic to ABO_3 families with e_g^1 occupation of the B-site *d*-orbitals, such as the 3-3 rare-earth manganites ($RMnO_3$) that present Jahn-Teller effect. DFT calculations predict that this polar phase can be strain-engineered in a few perovskites, such as $YMnO_3$, $SrTiO_3$, $BaMnO_3$ and $BiFeO_3$ [1]. We chose $SrTiO_3$ and $YMnO_3$, as they are the most promising to the purposes of this work.

In this work we are experimentally realizing challenging routes proposed in the literature that allow, via an applied E-field of 1 MV/mm, to control the MIT and electronic band gap of $YMnO_3$ and $SrTiO_3$ between 1.8 and 3 eV. For this, we used PLD to deposit epitaxial $YMnO_3$ and $SrTiO_3$ thin-films onto $LaMnO_3$ and MgO buffer layers deposited in Si, to reach a tensile strain between 3 and 5%, to stabilize the polar $Pb2_1m$ phase. This $Pb2_1m$ phase allows the coupling between the induced electric polarization and the OO mediated Jahn-Teller distortion. The E-field control takes advantage of the tailored coupling between the electric polarization and the OO associated distortion of the strain-engineered polar $Pb2_1m$ phase to control the physical properties by an applied E-field to the film. This work is funded by the PTDC/NAN-MAT/0098/2020 project.

[1] Phys. Rev. Lett. 116, 057602 (2016)
[2] Phys. Rev. B 98, 081108(R) (2018)

Combining Molecular Beam Epitaxy and Metal-Organic Chemical Vapor Deposition for GaInAsP-based Ultra-Wide Band Semiconductor Optical Amplifiers for device's performance optimization

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Keywords: Epitaxy, MBE, MOCVD, SOA, GaInAsP, Telecommunications

Molecular Beam Epitaxy (MBE) and Metal-Organic Chemical Vapor Deposition (MOCVD) are the main epitaxy techniques leading the III-V devices industry. Those two techniques have acquired a level of maturity allowing them to be operated as production tool. III-V Lab developed unique strategies combining the best of both worlds to significantly improve device performances.
As an example of such devices, Ultra-Wide Band Semiconductor Optical Amplifiers (UWB-SOAs), which are key in the design of next generation telecom networks have been manufactured by GasSource MBE (GS-MBE) for the base structure, including GaInAsP-based SL under-cladding and active region. The reactor is currently equipped with a full range of state-of-the-art *in situ* characterization tools such as the BandiT for accurate temperature measurement, a key parameter on InP. In addition, strain and stress measurement and control using EZ-Curve have been successfully operated during the growth of highly strained UWB-SOAs QWs.
After epiwafer processing, MOCVD's ability of growing high resistivity InP, doped with deep acceptors such as Fe or Ru to strongly reduce current leakage in devices has been put forward. A third epitaxy regrowth was then performed using either MOCVD or MBE, for the top cladding, and compare Zn and Be as InP p-type dopants, on device performances. The complete stack using the different techniques is shown on SEM picture figure 1.
This combination of both GS-MBE and MOCVD has been proven to fabricate high performance GaInAsP-based UWB-SOA in both O-band and C+L-band, with max gain of 21 dB and 31 dB respectively, covering their whole ranges of bandwidths.

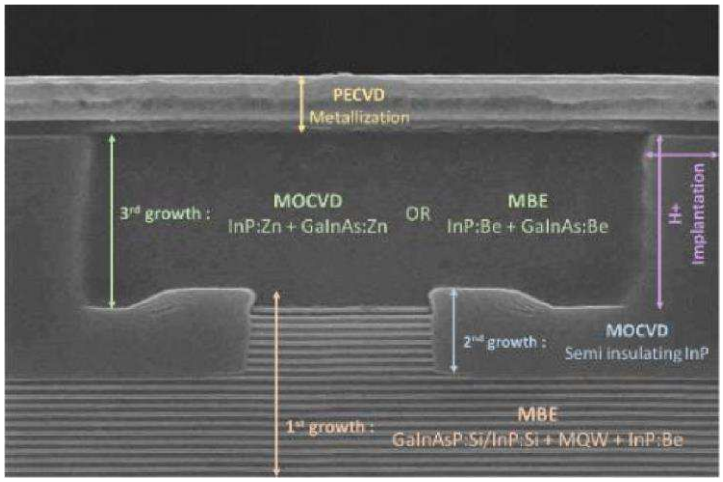

Fig. 1: Epitaxial structure of a typical UWB-SOA grown by MOCVD and MBE

Study on the epitaxial growth of WSe_2 on $PtSe_2$ sublayer

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Keywords: WSe_2, TMDC, epitaxial growth, CVD

Abstract: TMDs (Transition Metal Dichalcogenides) as MoS_2, WSe_2 etc., are layered van der Waals materials possessing relatively chemically inert surfaces. The lack of strong covalent bonds between a grown van der Waals material and a substrate significantly reduces the typical requirements for lattice matching in epitaxial growth and the integration of these materials into new technologies. This allows for the choice of materials systems based primarily on bandgaps and band offsets giving great flexibility in fabricating heterostructures with novel carrier confinement, carrier transport, and light emitting properties [1]. Here we present a new method to grow epitaxial WSe_2 films on SiO_2/Si substrates at relatively lower temperature with high repeatability and scalability. High quality crystalline films are achieved through direct selenization of deposited tungsten film with pre-deposited platinum as the underlayer. The self-assembled $PtSe_2$ layer, formed during selenization, assists the epitaxial growth of WSe_2. The crystallinity of the samples was determined by X-ray diffraction (XRD). Further characterizations with transmission electron microscopy (TEM), X-ray photoemission and Raman spectroscopy were conducted in order to assess the properties of the epitaxially grown structure.

Reference:
[1] Lee A. Walsh, Christopher L. Hinkle, van der Waals epitaxy: 2D materials and topological insulators, Applied Materials Today, Volume 9, pp 504-515 (2017)

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Remote Epitaxy of GaN via Graphene on GaN/Sapphire Templates

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Keywords: remote epitaxy, GaN, graphene, MOCVD

Abstract (Calibri, 11, 1-page max including eventual illustrations) Group-III nitrides are promising materials for next generation electronic and photonic devices. Extensive effort has been made to optimize group-III nitride heteroepitaxy for many years. However, inherent lattice mismatch and thermal expansion difference between nitrides and foreign substrates is still a limitation for GaN quality. The remote epitaxy of gallium nitride (GaN) via graphene has recently attracted significant attention as a new growth method which enables lift-of of GaN membranes. Yet, extensive research is still necessary to fully understand the III-nitrides formation on the van der Waals surface of 2D material and utilize remote epitaxy to its full potential.

In this work, the growth of the GaN epilayer using the GaN/sapphire template covered with graphene is presented. Metalorganic vapor phase epitaxy is chosen to fabricate both the template as well as the nitride epilayer on top as a cost-effective approach towards GaN homoepitaxy. One-step and multi-step growth temperature protocols are demonstrated while paying particular attention to the graphene interface[1]. GaN seeds formation on graphene is analyzed to identify remote epitaxy. Crystalline quality improvement of the epilayer by adjusting the growth parameters is further discussed to provide useful insights for GaN growth on a GaN/sapphire template via graphene.

The different graphene interlayer types for remote epitaxy of GaN was also studied[2]. Monolayer, bilayer, double-stack of monolayer, and triple-stack of monolayer graphene were transferred onto GaN/sapphire template using a wet transfer technique. The quality of the graphene interlayers was examined by Raman spectroscopy. The impact of interlayer type on GaN nucleation was analyzed by scanning electron microscopy. The graphene interface and structural quality of GaN epilayer were studied by transmission electron microscopy and X-ray diffraction, respectively. The influence of graphene interlayer type is discussed in terms of the difference between remote epitaxy and van der Waals epitaxy. Successful exfoliation of GaN membrane is demonstrated.

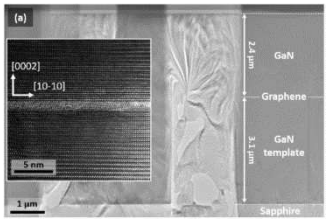

Figure 1: TEM images of GaN epilayers on graphene with the nucleation layer grown at different temperatures. Nucleation layer grown at 700C. Magnified GaN/graphene/GaN interface is shown in the inset.

References:

[1]K. Badokas, A. Kadys, J. Mickevicius, I. Ignatjev, M. Skapas, S. Stanionytė, E. Radiunas, G. Juška, T. Malinauskas, J. Phys. D: Appl. Phys. 54 205103 (2021).

[2]K. Badokas, A. Kadys, D. Augulis, J. Mickevičius, I. Ignatjev, M. Skapas, B. Šebeka, G. Juška and T. Malinauskas, Nanomaterials 12, 785 (2022).

In-situ microscopy: phase transformations during phosphorene formation on Cu(111)

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Keywords: 2D materials, phosphorene, in-situ microscopy, low energy electron microscopy, scanning tunneling microscopy

In-situ microscopy is a powerful tool to study early stages of materials growth. In this contribution, I will first introduce different approaches that aim to bridge the pressure gap between the growth reactors and an electron microscope. However, even ultra-high-vacuum studies provide valuable insights; this will be demonstrated on phosphorene growth on copper.
Phosphorene is one of the praised members of 2D materials family thanks to the exceptionally high carrier mobilities, predicted for both attractive 2D forms - black phosphorene and blue phosphorene. Unlike many other 2D materials, a monolayer of black phosphorus is strongly buckled and, thus, is not flat as e.g., graphene. Blue phosphorene exhibits much smaller buckling, yet still significant. Unlike black phosphorene, which can be exfoliated from bulk crystal, blue phosphorene results exclusively as a product of deposition on metal substrates. 2D materials are preferably grown on non-interacting substrates, as the interaction with the substrate may potentially result in spoiling of the desired properties and, potentially, prevent exfoliation. From this reason, the growth of (blue)phosphorene has been so far intensively studied on substrates predicted as non-interacting (hBN) or moderately-interacting (Au and Ag). It has been predicted by DFT simulation of phosphorene on different substrates that the weak (or non-existent) interaction leads to phosphorene stabilization, while the strong interaction results in breaking the phosphorene layer into separate nanodomains/clusters of phosphorus or metal phosphides.
On contrary, here we show that 2D phosphorus can be stabilized even on highly interacting substrate (Cu(111)) via series of unexpected phase transformations. Our data show that the copper phosphide phase is indeed formed, but it serves as a buffer layer for phosphorene formation. The related phase transformations are very rapid and point to the existence of a large "sea" of adatoms on the surface during deposition. We have been able to observe and monitor these transformations by concerted use of in-situ techniques, namely low energy electron microscopy (LEEM) and scanning tunnelling microscopy (STM). Our experimental results thus support recent theoretical predictions of these phase transformations playing significant role in formation of elemental buckled 2D materials.

The role of structural distortions in triggering the metal to insulator transition in $NdNiO_3$

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Keywords: Metal-to-insulator transition, structural transition, rare-earth nickelates, thin films

Rare-earth nickelates, $RNiO_3$, are challenging compounds due to their intriguing physics, consequence of the strong correlation between electronic, charge, spin and lattice degrees of freedom [1]. Among these compounds, $NdNiO_3$ has raised some controversy regarding the nature of its metallic to insulator transition (MIT). $NdNiO_3$ exhibits a first-order MIT, adopting a metallic and paramagnetic P*nma* symmetry above T_{MI} = 200 K and, in the insulating phase, transits into the $P2_1/n$ symmetry, with the stabilization of a E'-type antiferromagnetic phase [2]. In $RNiO_3$, a close relationship between structure and MIT has been proposed due to the strong dependence of the T_{MI} from the rare-earth cation size [3]. The symmetry lowering at MIT is supposedly accompanied by NiO_6 breathing distortion that once coupled to in-phase and anti-phase octahedra rotation distortions would trigger the MIT. However, contrarily to smaller rare-earth cations, in $NdNiO_3$, the amplitude of these oxygen rotations is not enough to stabilize the charge ordering and open the bandgap of the *eg*-Ni orbitals, and the magnetic ordering helps to promote the occurrence of MIT [3]. Therefore, in $NdNiO_3$, $T_{Néel} = T_{MI}$ is expected. While some experimental studies evidence the concomitant nature between structure and MIT [4], others completely reject it, assigning the magnetic ordering to the triggering mechanism instead [5]. The question still remains concerning the mechanisms that actual trigger MIT in $NdNiO_3$.

Towards searching for an answer to this demand, we have carried out an experimental study in $NdNiO_3$ ceramics and thin films of 260 nm and 110 nm deposited onto (001) oriented $LaAlO_3$ substrate by metal organic chemical vapor deposition. In this work, we report temperature-dependent Raman scattering and magnetization measurements to follow the structure and magnetic order evolution across the MIT, which was identified from resistivity measurements. The experimental results point out for a decoupling between the structural and electronic orders but evidence a coupling between electronic and magnetic orders in $NdNiO_3$, independently on the used sample type.

[1] G. Catalan, *Ph. Transit.* **81**, 729 (2008)
[2] S. Catalano et al., *Rep. Prog. Phys.* **81**, 046501 (2018)
[3] A. Mercy et al., *Nat. Commun.* **8**, 1 (2017)
[4] J. Y. Zhang et al., *Sci. Rep.* **6**, 23652 (2016)
[5] D. Meyers et al., *Sci. Rep*. **6**, 2793 (2016)

Epitaxy of hexagonal Ge-2H : growth regimes and related I3 defects

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Keywords: polytypism, step-flow, stacking faults, in situ TEM,

We present an in-situ growth study of the hexagonal Ge-2H crystal phase. GaAs nanowires with the wurtzite structure are used as template to create two kinds of heterostructures namely (1) core/shell and (2) trunk/branches. The growth is carried out using chemical vapor deposition with hydride precursors. Real time TEM observations at the atomic scale show the fundamental aspects of the epitaxy and the formation of growth-related staking faults in Ge-2H.

1) In core/shell configuration[1], the hexagonal crystal structure is transferred by epitaxy to the Ge shell. We show the different growth kinetics of Ge-2H on (1-100) lateral faces depending on temperature and precursor flow (figure1). We evidence the growth-related formation of original intrinsic stacking faults I_3 and discuss the correlation with the growth modes related to surface diffusion. A mechanism of I3 BSF formation is proposed.

2) The VLS and VSS growths of Au catalyzed Ge-2H branches[2], are observed on the (1-100) sidewalls of the GaAs-w nanowires with the <1-100> direction. The structure of those branches is presented and discussed (figure2).

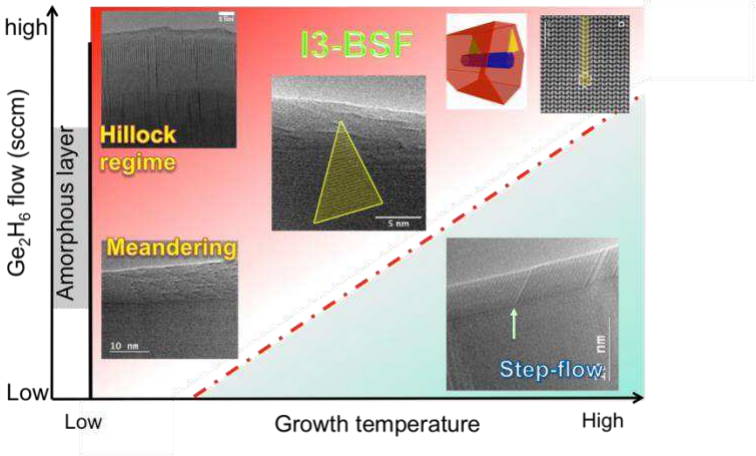

Figure1: growth kinetics of Ge-2H on GaAs-w (1-100)

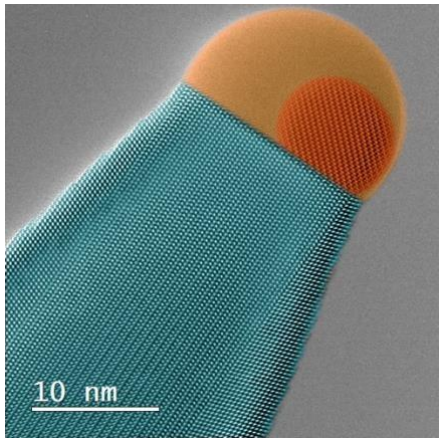

Figure 2: growth of <1-100>-oriented Ge-2H nanowire (partly solid Au catalyst)

[1] Growth-Related Formation Mechanism of I3-Type Basal Stacking Fault in Epitaxially Grown Hexagonal Ge-2H L. Vincent et al. Adv. Mat. Inter. 9-16 (2022) 2102340, *doi.org/10.1002/admi.202102340*

[2] Hexagonal Silicon-Germanium Nanowire Branches with Tunable Composition A. Li, H.I.T. Hauge, M.A. Verheijen, and E.P.A.M. Bakkers, R.T. Tucker, L. Vincent, C. Renard, Nanotechnology 34-1 (2022) 015601 *doi.org/10.1088/1361-6528/ac9317*

Molecular Beam Epitaxial Growth of SrMnSb2 Thin Films

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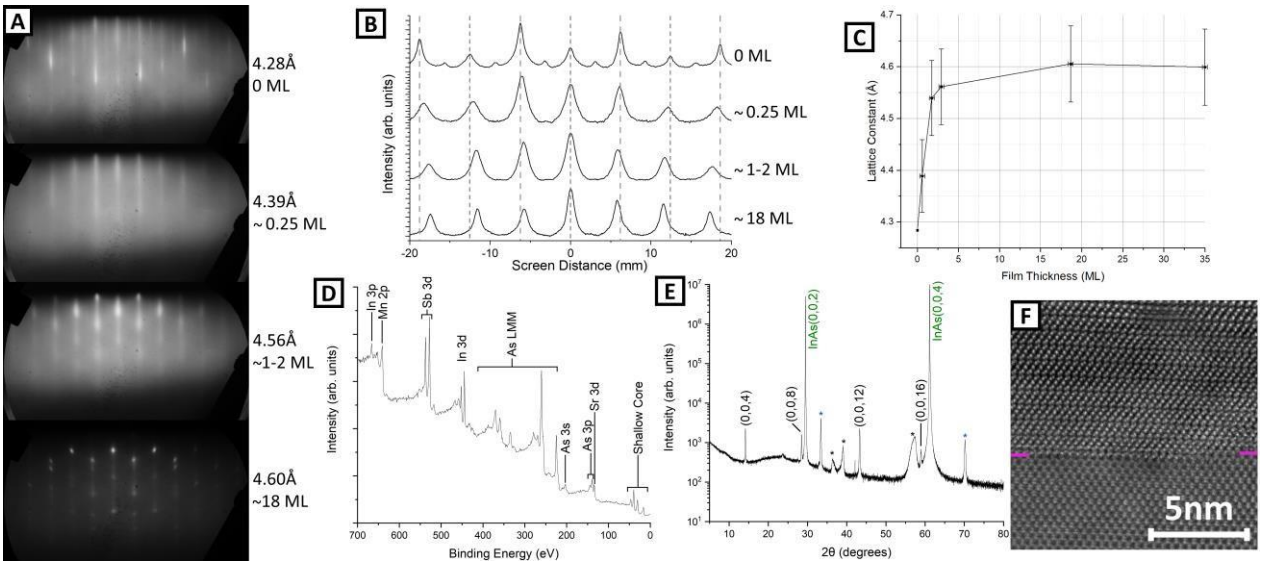
Keywords: MBE, Dirac semimetal, optoelectronics, thin films

MBE growth procedures have been developed to epitaxially grow the Dirac semimetal, $SrMnSb_2$, as a thin film with a protective As capping layer for ex-situ transfer and measurements. Studies of bulk material have returned evidence of Dirac fermions [1], but also predict a gap in the Dirac dispersion [2,3] that shows potential for optoelectronic devices but is as-yet unobserved. Additionally, strain induced by lattice mismatch on thin film samples are predicted to induce a change in the gap size [4] and films have been observed to relax to a larger than expected in-plane lattice constant. The films have been structurally and chemically characterised with a wide range of in vacuo and ex situ techniques, as exemplified in the figure. Growth optimisation and characterisation will be discussed in the presentation along with some of the challenges of MBE growth with the reactive metals Sr and Mn.



(A, B, C) RHEED images of thin film samples along the <110> direction at various thicknesses during growth, with intensity profiles and corresponding lattice constant measurements. (D) XPS data showing the composition of a $SrMnSb_2$ film after exposure to air and de-capping. (E) XRD of a capped sample showing out-of-plane $SrMnSb_2$ peaks (labelled) and InAs substrate peaks, where scattering from the As cap is weak and broad and unknown peaks (marked *) may come from endotaxial phases. (F) STEM of $SrMnSb_2$ film along <110> of the substrate, where pink dashes indicate the film/substrate interface.

[1] J. Liu *et al. Nature Mat.* 16, 905–910 (2017). DOI: 10.1038/NMAT4953.
[2] M. A. Farhan *et al., J. Phys.: Condens. Matter*, 26, 062201 (2016). DOI:10.1088/0953-8984/26/4/042201.
[3] C. P. Weber *et al., PRB 98,* 155115 (2018). DOI: 10.1103/PhysRevB.98.155115.
[4] [4] N.R. Wilson, *et al. Nano Res.* 6, 99, (2013). DOI 10.1007/s12274-013-0285-y

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Congruent evaporation of $CsPbBr_3$ perovskite studied by Knudsen Evaporation Mass Spectroscopy

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Keywords: perovskite, $CsPbBr_3$, Knudsen Effusion Mass Spectroscopy

Hybrid organic-inorganic lead halide perovskites (MAPbX3, MA – methylammonium, X – halogen) are the most frequently studied types of perovskites. They possess properties that make them ideal for various optoelectronic applications, such as ionizing radiation detectors and photovoltaic cells, with efficiencies exceeding 20%. However, one major drawback is their sensitivity to external influences such as oxidative atmosphere, UV radiation, high temperatures, and humidity, which can cause degradation of their properties. This sensitivity is typically attributed to the organic component of the perovskite, and the preparation of a completely inorganic perovskite is seen as an obvious solution to suppress these effects.

An example of a fully inorganic perovskite is CsPbBr3, which retains properties suitable for optoelectronic applications and is highly sensitive to high energy radiation. It is believed to be a suitable replacement for existing materials used in detectors.

Despite the varying process conditions or precursors used, the final product always has a CsPbBr3 stoichiometry. The evaporation process can be done using a single source such as a CsPbBr3 powder or pellet, co-evaporation of multiple precursors like CsBr and PbBr2 powders, or even a sequential process with extra annealing steps after deposition. It is generally supposed that the evaporation process of these compounds is congruent and results in correct stoichiometry of the final compound. However, this is not based on any exact scientific evidence.

We have evaluated the evaporation products using Knudsen Effusion Mass Spectrometry. This method combines a Knudsen effusion cell with a mass spectrometer, where the vapor from the cell is directed as a molecular beam through an orifice into the mass spectrometer. The result of the analysis provides information about the partial pressures and the composition of the vapor. Furthermore, we compare the data with photoluminescence spectra and electron micrographs.

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