

## Ferroelectric Topological Structures in Epitaxial Layers

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Contribution: Oral

Ferroics can form complex topological spin structures such as vortices and skyrmions, especially when subjected to particular boundary conditions. In ferroelectrics vortex-like electric dipole- based topological structures have been observed in dedicated ferroelectric systems, especially PbTiO<sub>3</sub>/SrTiO<sub>3</sub> ferroelectric/insulator superlattices, which have proven to be an ideal model system due to their high depolarising field. The large electrostatic energy is minimised by local rotations of surface dipoles, similar to ferromagnetic Kittel domains, in the which local dipoles rotate in such a way to reduce both the depolarization and stray fields, avoiding the suppression of the ferroelectricity in the thin films.

In single PbTiO<sub>3</sub> epitaxial layers sandwiched between SrRuO<sub>3</sub> electrodes we observe a more complex domain structure analogue of the double- $\vec{Q}$  magnetic spin crystal phase. This comprises of periodic clockwise and anti-clockwise ferroelectric vortices which are modulated by a second cycloidal ordering along their toroidal core. Thus, one  $\vec{Q}$  vector determines the periodicity of vortices and a second  $\vec{Q}$  vector breaks the uniformity of the domains in the perpendicular direction, leading to a state described by a double- $\vec{Q}$  modulation. The interplay of only two orthogonal periodic modulations results in the so-called incommensurate spin crystal. [1]

The presence of such a double- $\vec{Q}$  structure, mediated by incommensurate interactions, would require an electric counterpart of the magnetic Dzyaloshinskii-Moriya interaction (DMI). Such an electric DMI could provide the phenomenological explanation of the emergence of magnetic-like phases in ferroelectric systems.

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## Combinatorial pulsed laser deposition for interface engineering in ferroelectric capacitors

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Keywords: combinatorial pulsed laser deposition, LaSrMnO<sub>3</sub>, BaSrTiO<sub>3</sub>, interface control

Contribution: Oral

Abstract:

We will present the development of a combinatorial pulsed laser deposition (CPLD) oriented towards interface engineering in perovskite heterostructures. Interface Control Layer (ICL), proposed for Si and GaAs based heterostructures [1], is one of the possible strategies for band structure engineering at the metal / semiconductor interface. By CPLD the interface composition can be continuously modulated on a few atomic layers, thus giving access to a library of ICL materials in one single sample. The modulated ICL is fabricated by successive depositions from two different target materials. Appropriate control of the deposition rate assures the composition control at the unit cell level, and a moving shadow mask distributes the material deposited from each target across the substrate surface in order to vary locally the composition. The result of this CPLD process is a film that has a continuous variation of the in-plane composition (between those of the two targets) along one direction of the sample [2].

We will demonstrate that a La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> (LSMOx) ICL inserted between La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> (LSMO) electrode and SrTiO<sub>3</sub> (STO) film in an epitaxial heterostructure modulates the band bending at the LSMOx / STO interface and induces a continuous tuning of the electric contact nature from Schottky to ohmic. The same LSMOx ICL implemented in polycrystalline Pt / LSMOx / (BaSr)TiO<sub>3</sub> / Au heterostructure on Sapphire influences both the tunability and losses. XPS/UPS spectroscopies used to probe core levels, work function (WF), and band bending versus composition will be presented, as well as local I(V)s measurements by UHV AFM in contact mode through the interfaces and macroscopic impedance spectroscopy results.

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## **Exploring the Influence of Non-Ferroelectric Elements on Polarization Switching in Ferroelectric Devices: Towards Understanding and Controlling Dynamic Behavior**

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Keywords: negative capacitance, ferroelectrics, switching dynamics, epitaxial multilayered structures, polarization compensation

Contribution: Oral

Abstract :

Ferroelectricity, discovered over a century ago, has found numerous applications based on its ability to change polarization using an external electric field. These applications include ferroelectric random access memory (FERAM) and ferroelectric field-effect transistors (FEFET). The dynamics of polarization switching are crucial for binary digital devices, influencing parameters such as writing speed, voltage, stability, and fatigue. Intermediate polarization states have been explored for memories with multiple states and analog or neuromorphic computing. Additionally, integrating ferroelectric layers into field-effect transistors has introduced the concept of negative capacitance (NC), enabling power consumption reduction beyond the thermodynamic limit. However, achieving the NC regime involves non-equilibrium conditions during the ferroelectric system's transition. Despite employing various methods to control switching dynamics, further research is needed to understand the intricate relationship between polarization switching in ferroelectrics and external electrostatic conditions.

The study highlights that the nature of non-ferroelectric (non-FE) elements, whether resistive or capacitive, can significantly influence switching characteristics, often overlooked in conventional measurements. The study aims to introduce a simple methodology for investigating the impact of imperfect screening or charging/discharging phenomena on polarization switching in thin and ultra-thin ferroelectric films and multilayers. By connecting commercially acquired resistors and capacitors in series with high-quality epitaxial ferroelectric capacitors, the study analyzes the influence of non-FE element resistivity and polarizability on nonlinear polarization switching behavior. The distribution of applied voltage across different components is analyzed during the ferroelectric switching process, revealing varying characteristics of negative capacitance (NC) regimes depending on the non-FE element. Moreover, intentionally delaying polarization charge compensation during switching induces a non-equilibrium regime in the ferroelectric layer.

The electrical characterization is conducted on a 200 nm thick layer of PbZr<sub>0.2</sub>Ti<sub>0.8</sub>O<sub>3</sub> (PZT) deposited on SrTiO<sub>3</sub> (001) (STO) substrates, with a 20 nm SrRuO<sub>3</sub> (SRO) layer serving as the bottom electrode, using pulsed laser deposition (KrF excimer laser). Additionally, two bilayer structures are created by depositing 20 nm of non-ferroelectric (non-FE) materials (Nb-doped STO-STON or Ba<sub>0.4</sub>Sr<sub>0.6</sub>TiO<sub>3</sub>-BST) on top of the two PZT structures.

## Epitaxial ferroelectric thin films and their potential for energy storage

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Keywords: epitaxy, ferroelectrics, thin films, energy storage

Contribution: Oral

Dielectric capacitors offer significant advantages for energy storage materials because of their high power density, high storage efficiency, operating temperature, cycling stability, and quick charging and discharging times. The issue with dielectric materials is that they have a low energy storage density (ESD) compared with batteries. Here, the research has focused on developing the electrostatic solid-state supercapacitors from electrically polarizable materials such as ferroelectrics. The most typical characteristic of such materials is the significant nonlinear relationship between polarization (P) and applied electrical field (E), which is defined as the P-E loop. Fig. 1 makes a suggestion regarding the association between the P-E loop and energy storage density. A thorough comprehension of the physics governing the P-E loop's behavior is necessary for the design and optimization of such devices, and this requires epitaxial structures obtained on monocrystalline substrates such as strontium titanate (STO). According to our preliminary findings, epitaxial ferroelectric materials continue to be a promising approach for the development of next-generation energy storage systems.

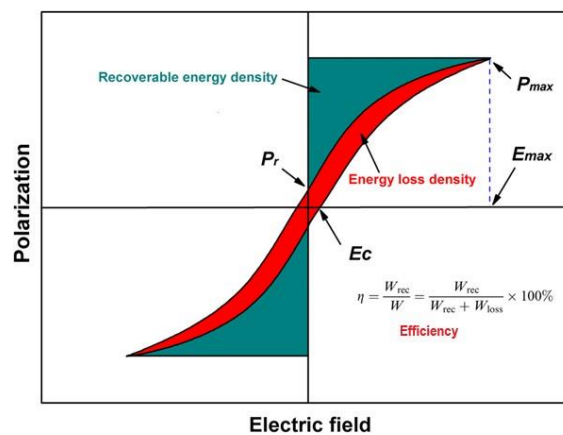


Fig.1. The relationship between P-E loop and energy storage density

## Novel 2D materials for neuromorphic computing

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Keywords: Resistive Switching, 2D Materials, Neuromorphic Computing

Contribution: Oral

In recent years, atomically thin two-dimensional (2D) van der Waals (vdW) layered transition metal dichalcogenides (TMDs) have attracted significant attention due to their excellent electronic and optoelectronic properties.<sup>1</sup> Especially, metallic TMDs (e.g., NbS<sub>2</sub>, NbSe<sub>2</sub>, TaS<sub>2</sub>) have shown exotic physical properties such as superconductivity and charge density waves. However, due to the poor stability in ambient conditions, fabricating high performance devices with long lifetime, is still a huge challenge. In most of these metallic TMDs, the formation of native oxide is unavoidable. Thus, this oxide is being exploited to produce scalable, flexible, and transparent metal-insulator-metal devices for neuromorphic and memory applications.<sup>2,3</sup>

Here, we propose the Au/NbSe<sub>2</sub>/NbO<sub>x</sub>/graphene memristive heterostructure, in which oxygen vacancies form conductive filaments under applied electrical potential. Both NbSe<sub>2</sub> and graphene were mechanically exfoliated and NbSe<sub>2</sub> is intentionally oxidized to get a layer of NbO<sub>x</sub> by heating it at 80°C for a few minutes in ambient conditions (Fig. 1). We obtained bipolar resistive switching with a stable low/high-resistance-state ratio of 10<sup>3</sup> and endurance over more than 500 cycles. Furthermore, we observed potentiation and depression under millisecond applied pulses. This work will open new opportunities for next-generation neuromorphic scalable devices.

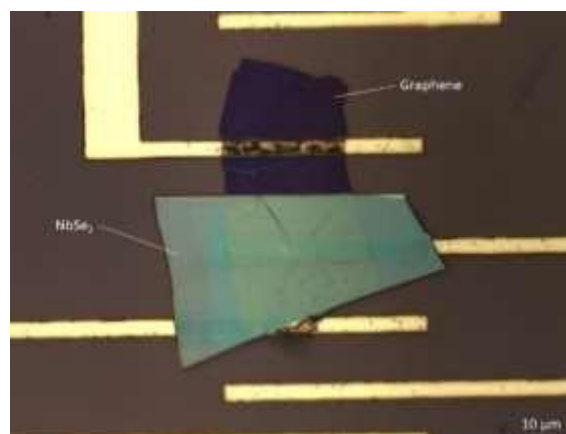


Figure 1: Optical image of the fabricated Au/NbSe<sub>2</sub>/NbO<sub>x</sub>/graphene device.

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## Optimization of Semiconductor-Superconductor hybrid systems for the development of Andreev qubits

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Keywords: Andreev qubits, 2DEG,

AluminumContribution: Oral

Two-dimensional electron systems confined near the surface of narrowband semiconductors integrated with superconductors lay the foundations of a radically new hybrid solid-state platform for scalable quantum computing based on Andreev quantum bits (qubits)<sup>1</sup>. To this aim, InAs 2D electron gases (2DEGs) are among the ideal semiconductors for these systems due to their vanishing Schottky barrier; however, their exploitation is limited by the non-availability of commercial lattice-matched substrates<sup>2,3</sup>.

Here, we demonstrated in-situ growth of aluminum films on near-surface InAs 2DEGs can be grown by Molecular Beam Epitaxy on GaAs substrates with quality comparable to state-of-the-art growth on InP despite 7% InAs/GaAs lattice mismatch<sup>4</sup>. To optimize electron mobility in the 2DEG, we identified the main scattering mechanisms in gated Hall bar structures developed within a STSM, and with the help of a theoretical model. Also, superconducting proximity effect was observed in Josephson junctions. The developed growth protocol could thus set a new standard for the fabrication of Andreev qubits on GaAs technology.

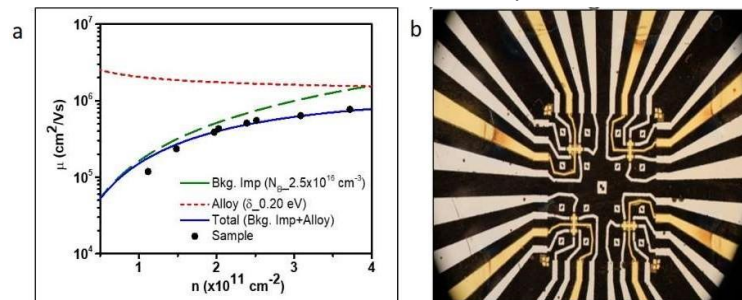


Figure 1a) Mobility versus carrier density curve of a gated hall bar on 130nm deep quantum well structures fitted with the total scattering mechanism curve. b) Optical microscope image of hall bars fabricated on these structures.

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## Synthesis and Characterization of HOPG-Thin metallic films

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**Keywords:** HOPG, Deposition, Thin Films, Morphology, XPS,

**Contribution:** Oral

### Abstract

Highly oriented pyrolytic graphite (HOPG) is an exceedingly ordered form of synthetic graphite, and it is currently widely regarded as one of the most important materials as a substrate for nanoscale applications. HOPG is very smooth, inert, has metallic qualities hence no or less surface charging issues and can be cleaved easily to provide a fresh surface.

The current study aimed to fabricate the HOPG-metallic (M) thin film systems through the electron beam physical vapour deposition (EBPVD) technique. High-purity (99.9%) titanium (Ti), silver (Ag) and gold (Au) were deposited on HOPG (Dimensions: 5 x 5 x 1 mm) to form HOPG-M thin films with a nominal thickness of 10 nm under a high vacuum environment. The three materials were selected based on their important applications in different fields such as catalytic activities and surface plasmon resonance. The Bestec evaporator system is equipped with a quartz-crystal mass-thickness sensor used for the measurement of the thickness of the deposited layer and regulation of the deposition rate.

The prepared HOPG-thin films were subjected to characterization to investigate their properties. Surface morphology from scanning electron microscopy (SEM) shows that HOPG-Ti film had a smooth and crack-free surface, while HOPG-Au and HOPG-Ag films formed films with nano-cracks. Different morphologies show that the growth mechanism for the thin films was different. Topographical features from atomic force microscopy (AFM) showed that HOPG-Ti had uniform and flat film, HOPG-Au had densely, and uniformly distributed islands and HOPG-Ag had randomly and less dense islands. The surface roughness was 0.44, 0.55 and 1.12 nm for HOPG-Ti, HOPG-Au and HOPG-Ag respectively. X-ray photoelectron spectroscopy (XPS) shows that Ti film existed in both metallic and oxidized states while Au- and Ag films were in the metallic state. The surface of the HOPG-M thin films exhibits oxygen-containing moieties such as hydroxyl, carbonyl, and carboxylic groups. Raman spectroscopy established that HOPG-M thin films showed G and 2D modes of vibration and established the presence of the other vibrations at low frequencies due to O-Ti-O and Au and Ag lattice phonons.

It is believed that the obtained results will find application in the determination of the most appropriate parameters (composition, thickness) for the deposition of the M thin films. The results provide a deeper understanding of crucial parameters related to the future design of electronics, optics, biosensors, and other devices using M thin films deposited on the HOPG substrate. This work also provides an opportunity for further examination of the HOPG as a substrate for the preparation of different M thin films.

## Development of customized GaAs-based terahertz quantum-cascade lasers

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Keywords: Terahertz quantum-cascade lasers, in-situ growth control

Contribution: Oral

Terahertz (THz) quantum-cascade lasers (QCLs) are compact and powerful radiation sources emitting in the frequency gap between electronic microwave emitters (up to about 1 THz, 300  $\mu\text{m}$ ) and infrared semiconductor lasers (starting at about 30 THz, 10  $\mu\text{m}$ ) where many rotational transitions of molecules and fine structure transitions of atoms occur. Thus, THz QCLs can be applied for high resolution spectroscopy of gases or plasmas in lab reactors or in the atmosphere and for astronomic research. However, the requirements of these applications are not trivial to fulfil and include an optical output power of typically at least 1 mW, a working temperature as well as a wall plug efficiency to be compatible with miniature mechanical cryocoolers, and a high stability of emission frequency and power.

THz QCLs have been fabricated at the PDI now for more than 15 years, where we have the possibility to work on each development stage in-house, which comprises the sophisticated design and simulation of the layer structure [1] and waveguide properties, the MBE growth, lithographic processing and setting up functional laser bars, and characterization of structural quality and laser performance. Consequent iteration processes can be efficiently implemented according to the results and may induce changes in the design, in the processing, or in the MBE growth process.

Our typical THz QCLs consist of 70 to 120 periods, which, in principle, allows for emission of a photon in every period of the cascaded structure triggered by a single charge carrier. These numbers of periods add up to more than 1000 individual layers and an overall thickness exceeding 10  $\mu\text{m}$ . At our typically applied growth rate of 0.13 nm/s, the overall growth time amounts to about 24 hours. To meet the requirements of layer thickness precision and also to ensure a constant growth rate during these long deposition times, we established a closed-loop automatic control setup based on continuous spectral reflectivity measurements [2]. Resulting run-to-run thickness variations measured at the center of two-inch wafers are much smaller than the radial decrease of the thickness, which is given by the geometry of the growth chamber. The latter can be measured ex-situ, and by feeding this data into the simulation model, we can determine the radial position on the wafer that will lead to devices emitting at the desired target frequency [3].

The possibility to cover all stages under one roof allows for efficient development of customized THz QCLs for applications like local oscillators in heterodyne receivers for astronomy [4], gapless time-averaged wideband emitter as powerful source in absorption setups [5], or emitters that can be tuned across ion absorption lines for high-resolution plasma spectroscopy [6].

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## **Surface charge effects in GaN NWs: An advantage for enhancing the piezoelectric conversion efficiency**

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Keywords: GaN NWs, Surface charge effects, Piezo-nanogenerators, Energy harvesting

Contribution: Oral

### Abstract

Piezoelectric nanowires (NWs) are promising to develop ultra-compact and high-efficient piezo-nanogenerators working under environmental conditions for supplying micro-devices. Especially sub-100 nm-wide NWs exhibit properties strongly different from bulk or micrometric structures, that lead to a modulation of their characteristics favorable for piezoelectric generation. Among them, we can cite the surface charge (SC) effects. Simulations have predicted that in given conditions, the SC effects can be advantageous for improving the piezo-response. In-depth understanding of the relationship between the SC and the piezo-conversion capacities of the NWs is now a prerequisite for further improving the device performances and thus approaching a future technological transfer.

To experimentally quantify the influence of the SC on the piezo-response of the GaN NWs, we have combined new advanced nano-characterization tool based on AFM probing the piezoelectric properties of NWs axially compressed and Time-Resolved PL measurements.

The expression of the SC effects being strongly linked to the NW diameter [1], we have quantified the piezo-generated output voltages and the electromechanical coupling coefficient of GaN NWs characterized by diameters evolving between 20 and 110 nm. We established that the piezo-response of the NWs is strongly affected by the SC effects. While for large diameter (60 nm in the intrinsic doping conditions of our NWs), the SC do not affect the NW piezo-conversion, for lower diameters, the SC effects become favorable. We evidence an enhancement of the piezo-response of the NWs due to the strong reduction of the screening effect of the piezo-charges into the fully depleted NWs. Especially, we demonstrate that by finely architecting the NWs dimensions, the SC effects are advantageous for strongly improving the electromechanical conversion efficiency of GaN NWs up to 43,2% [2].

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## How Can InGaN/GaN Heterostructures Be Advantageous for the Piezoelectric Conversion of GaN Nanowires and their Applications?

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Keywords: Gallium Nitride, Nanowires, Energy Harvesting, Piezoelectricity

Contribution: Oral

Abstract (The IoT demands for smart, integrated, miniaturized and low-energy wireless devices are constantly on a rise both in our daily life and in high-tech applications and the question of their energy supplying is now a key worldwide challenge. Nanowires (NWs)-based piezoelectric nanogenerators have appeared these last years as a new solution for replacing the batteries by converting the environmental vibrations into electrical energy. While these new energy sources have demonstrated power densities in the  $\mu\text{W}$ - $\text{mW}/\text{cm}^3$  range, their use as micro-system power supply working under environmental conditions remains today rather limited. To consider them for supplying micro-devices, the improvement of the conversion efficiency per surface unit of the piezoelectric active layer is a pre-requisite. We demonstrated that by integrating  $\text{In}_{0.35}\text{Ga}_{0.65}\text{N}$  thick homogeneous insertion in the GaN NW volume, we improved the piezoelectric response of the GaN NWs [1] due to the higher piezoelectric coefficients of InGaN [2].

An increase of the power density of about 20% in presence of InGaN is highlighted, both at nano- and macro-scales studied under environmental-like solicitation conditions (few Newton 1-100 Hz). At macro-scale, a maximum power density of  $3.1 \mu\text{W}/\text{cm}^2$  ( $23.1 \text{ mW}/\text{cm}^3$ ) was reached under intermittent contact solicitation, with a maximum peak-to-peak output voltage attaining 143 mV. This enhancement allows us to approach the power requirements of microelectronic systems, such as medical implants ( $1\mu\text{W}$ - $10\mu\text{W}$ ).

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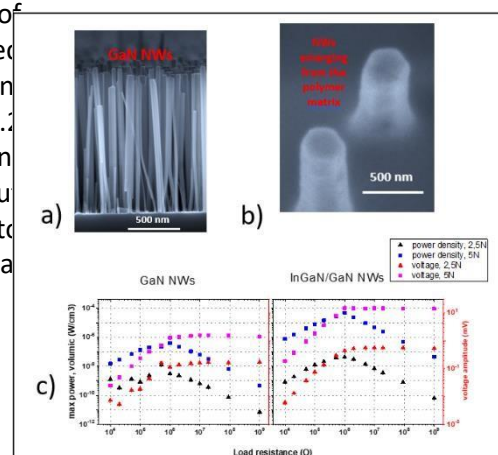


Fig. 1. SEM images of GaN nanowires (a)) and GaN NWs emerging from the polymer matrix (b)), Load resistance-dependent response of an InGaN/GaN NW-based transducer under 210 Hz permanent sinusoidal solicitation (c)).

## DC current-voltage and impedance spectroscopy characterization of CdS/ZnTe heterostructures

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Keywords: CdS/ZnTe, heterostructure, diode factor, current transport, impedance, minority carrier lifetime, acceptor impurity density.

Contribution: Oral

### Abstract

In this paper, we have investigated current transport across CdS/ZnTe heterojunctions fabricated by close space sublimation method using conventional DC current-voltage (I–V) measurements and impedance spectroscopy by choosing proper equivalent circuit models. The transparent frontal contact were deposited on glass substrates by DC magnetron sputtering from ZnO:Al:Cl target. CdS and ZnTe powders of 99.999% purity were purchased from Alfa Aesar, Germany. For synthesizing CdS and ZnTe thin films closed-space sublimation method (CSS) was developed. The deposition temperatures for the ZnTe thin films were chosen to prevent re- evaporation of the CdS thin films. The CdS and ZnTe thin films of thickness  $\sim 234$  nm and of  $\sim 3.07$   $\mu\text{m}$ , respectively were grown on conductive ZnO substrate. As a back contact was used Ag paste treated at 50 °C for 30 min. DC current-voltage characteristics were measured using a Keithley 2400 source measuring unit using voltage sweep mode. AC impedance measurements were carried out using an HIOKI 3532-50 LCR impedance analyzer at frequencies ranging from 100 Hz to 3 MHz by applying a sinusoidal voltage having 0.2 V. Complex impedance measurements of the CdS/ZnTe, temperature range from 220 K to 350 K and over the frequency range from 50 Hz to 16 kHz.

The dark I-V characteristics of CdS/p-ZnTe heterojunctions were measured over a wide (220-350 K) temperature region. From these dependencies, the reverse saturation current ( $I_s$ ), the barrier height ( $V_{bi}$ ) and the ideality factor ( $n$ ) were estimated. The barrier height values change chaotically from 0.87 eV to 1.11 eV in the temperature range (220-350) K without obeying the law. The values of the ideality factor decreased from 3.6 to 2.1 with increasing temperature from 220 K to 280 K, and then until 350 K changes very slightly around the value of 2. The activation energy of the carriers calculated from the slopes of the straight lines  $\ln I_s = f(10^3/T)$  produces values of  $\Delta E_a = 2.1$  meV and 66.4 meV, respectively. From C-V measurements we found the impurity ( $N_{ef}$ ) concentration of the carrier's order of  $10^{17}$ . The depleted capacitance obtained at zero bias for the CdS/ZnTe structure changes slightly with temperature. The frequency dependence of the real  $Z'$  and the imaginary  $Z''$  of the complex impedance at different AC-voltages shows that at lower frequencies, the  $Z'$  and  $Z''$  values increase with increasing the applied AC-voltage. The capacity shows a relaxation maximum in the vicinity of the frequency of 1 kHz, followed by a monotonous decrease with frequency. The loss trend shows high values at both low frequencies below 1 kHz and at high frequencies above 1 MHz, keeping subunit values in the intermediate region. The Nyquist plots show the presence of bulk and grain boundary effects in the system. Each semicircle is a representative of RC circuit that corresponds to individual component of the material. The increase in temperature influences the conductivity values recorded at low frequencies. They vary according to an Arrhenius-type law with a change in slope for two temperature segments with activation energies of  $\sim 28$  meV at low temperatures and  $\sim 64$  meV at high temperatures. By exploring DC current-voltage characteristics and impedance spectroscopy, a variety of properties can be separately investigated, including transport in the photoactive layer, contacts, bulk or surface capacitance.

## Optimizing the properties of $\text{CaMnO}_3$ for thermoelectric applications through Laser Floating Zone processing

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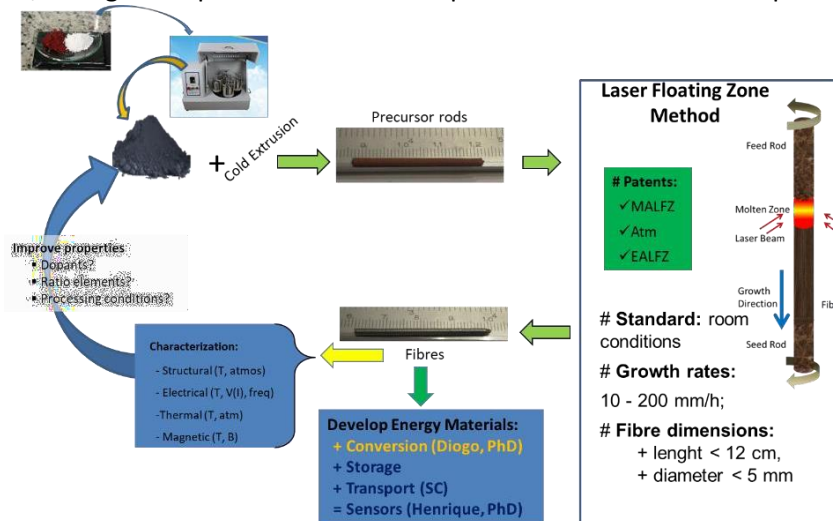
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Keywords: thermoelectric material,  $\text{CaMnO}_3$ , laser processing

Contribution: Oral

Abstract:

Electroceramics materials present unique properties, which depend on their composition and processing technique. This oxide presents stability at high temperatures and allows tuning of the relevant electrical and thermal transport properties through doping. In this work,  $\text{CaMnO}_3$  doped with different oxides have been prepared to produce fibres through the laser floating zone technique using different pulling rates and conditions (atmospheres, an external electrical or magnetic field). Particular emphasis is given to LFZ processing under a magnetic field, allowing unique opportunities for tuning the structural, microstructural and magnetic properties. This technique allows the growth of fully dense fibres, as well as the formation of metastable phases and/or promoting different oxidation states by adjusting the growth conditions. The results demonstrate some guidelines for tuning the phase composition and microstructure by adjusting the growth conditions. The effect of the magnetic field applied during the growth produces different effects in the phases formed and thus the magnetic performance of the samples, which allows a potential phase tuning of these materials. The obtained guidelines suggest that LFZ is a suitable technique for processing oxides if optimized control, over growth parameters and re-equilibration conditions is imposed.



## Controversial issues and challenges pertaining to the growth and properties of Cu<sub>2</sub>O

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Contribution: Oral

Abstract:

Cuprous oxide (Cu<sub>2</sub>O) is a p-type metal-oxide semiconductor that has a fundamental, direct energy bandgap of 2.1 eV and cubic crystal structure. The native p-type conductivity of Cu<sub>2</sub>O is related to the occurrence of acceptor-like copper vacancies ( $V_{Cu}$ ). Cu<sub>2</sub>O has been suggested to be suitable as a solar cell absorber for a long time but device efficiencies have been limited so far to less than 10% <sup>1</sup>. Nevertheless, it is an active topic of investigation for the fabrication of solar cells and photocatalysis but also for CO<sub>2</sub> reduction. Cu<sub>2</sub>O has also been used as an archetype for the study of Rydberg excitons with very large principal quantum numbers of  $n = 25$  and giant wavefunction extensions in excess of 2  $\mu\text{m}$  in gem crystals of Cu<sub>2</sub>O <sup>2</sup>. More recently Rydberg exciton-polaritons were detected in a SiO<sub>2</sub>/Ta<sub>2</sub>O<sub>5</sub>/Cu<sub>2</sub>O/Ta<sub>2</sub>O<sub>5</sub>/SiO<sub>2</sub> Fabry-Pérot cavity using natural gem Cu<sub>2</sub>O <sup>3</sup>.

Here I will describe how it is possible to obtain Cu<sub>2</sub>O layers that do not contain Cu<sub>4</sub>O<sub>3</sub>, CuO or Cu that is critical for the observation of excitons in Cu<sub>2</sub>O layers but also for the fabrication of solar cells. Furthermore, I will show that Cu<sub>2</sub>O layers obtained under optimum conditions exhibit a detailed spectral structure and distinct peaks at 2.75, 2.55 and 2.21 eV corresponding to the blue, indigo and yellow direct transitions of Cu<sub>2</sub>O as observed by ultrafast pump-probe spectroscopy at room temperature. A lower energy transition at 1.8 eV is attributed to carrier recombination via states located  $\sim 0.4$  eV below the conduction band whose origin remains controversial and is discussed in conjunction with electronic structure calculations as it is very important from an applied and fundamental point of view.

### References

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<sup>2</sup>T. Kazimierczuk *et al.* "Giant Rydberg excitons in the copper oxide Cu<sub>2</sub>O," *Nature* **514**(7522), 343–347 (2014).

<sup>3</sup>K. Orfanakis *et al.* "Rydberg exciton–polaritons in a Cu<sub>2</sub>O microcavity," *Nat Mater* **21**(7), 767– 772 (2022).

## **Giant room temperature magnetoresistance of unrelaxed La.<sub>0.67</sub>Ba.<sub>0.33</sub>Ti.<sub>0.02</sub>Mn.<sub>0.98</sub>O<sub>3</sub> epilayers grown on 001-oriented SrTiO<sub>3</sub>**

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Keywords: epitaxy; GMR; RT PM-FM phase transition

Contribution: Oral

Several manganites possess large RT-GMR and considering that the highest GMR occurs at  $T_C$ , manganites with  $T_C$  as close as to RT should be envisaged and engineered for potential room temperature applications. La.<sub>0.67</sub>Ba.<sub>0.33</sub>MnO<sub>3</sub> (LBMO) has a  $T_C \sim 343\text{K}$ , while the partial substitution of Mn with the not-carrying magnetic moment Ti decreases the  $T_C$ .

The pseudocubic lattice constant of LBMO is  $3.908 \text{ \AA}$ , favoring the epitaxial growth on the SrTiO<sub>3</sub> (STO) 100 surface, due to extremely low lattice mismatch ( $a_{\text{STO}} = 3.905 \text{ \AA}$ ). Doping with Ti (2%), the lattice constant of La.<sub>0.67</sub>Ba.<sub>0.33</sub>Ti.<sub>0.02</sub>Mn.<sub>0.98</sub>O<sub>3</sub> (LBTMO) increases to  $3.912 \text{ \AA}$ , while the calculated critical thickness (the thickness up to which relaxation does not occur) is above 200 nm.

Films of 100 nm are obtained by ablating a LBTMO ceramic target onto STO 100 terraced surface. There is a structural transformation from the rhombohedral lattice of the target to the cubic/tetragonal one of the film due to the characteristics of the monocrystalline substrate, leading to an out-of-plane lattice parameter of  $3.928 \text{ \AA}$ . The tetragonality of the crystalline structure is sustained by the selected area electron diffraction profiles along [100] and [001] directions.

The PM-FM phase transition can be estimated as the intersection point of the two tangents to the isofield curve that bounds the transition temperature ( $T_C^t \sim 295\text{K}$ ) or as the extreme value found by representing the temperature dependence of the magnetization derivative ( $T_C^d \sim 286\text{K}$ ). The  $T_C$  value is slightly smaller than the 309K one of powdered sample.

The temperature dependencies of the film resistivity in zero and 5 Tesla external magnetic fields were measured by using a linear geometry, while the magnetic field is perpendicular to the *ab* plane of the film and consequently to the current direction. In the external magnetic field, the conductivity increases significantly in the vicinity of  $T_C$ , thus the metallic-like character is kept up to the highest achievable temperatures. The external magnetic field assists the hopping of  $e_g$  electrons between neighbour Mn ions (from occupied to non-occupied lowest energy states), while a higher temperature increases the relative number of occupied  $e_g$  states of lowest energy. Giant magnetoresistance as high as 60% at room temperature (using the resistance values in a field of 5 Tesla) was recorded for the LBTMO epilayers being the highest one reported until now on such oxides.

Reference: Applied Physics Letters 111, 182409 (2017), <https://doi.org/10.1063/1.4998011>

## Metal exsolution dynamics and thermal stability limitations of exsolved nanoparticles at complex oxide surfaces

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Wolfgang Rheinheimer<sup>3,6</sup>, Regina Dittmann<sup>2</sup>, Rainer Waser<sup>2,7</sup>, Olivier Guillon<sup>3,6,8</sup>, Stephen J.  
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**Keywords:** Metal exsolution, Oxide epitaxy, Nanostructured catalysts, Supported nanoparticles, Solid oxide cells  
**Contribution:** Oral

**Abstract:** One-step metal exsolution reactions enable the synthesis of nanostructured catalysts based on the release of dopants from parent oxides upon thermal reduction. The concept of metal exsolution can be used to functionalize perovskite oxide electrode materials for the application in energy conversion devices, such as solid oxide cells. Here, exsolved nanoparticles may serve as catalytic centers for electrochemical conversion reactions, where a high robustness of the supported nanoparticles with respect to coarsening is crucial for the design of durable exsolution catalysts.

The mass transfer kinetics of the reducible dopants from the near-surface region of the oxide parent to the oxide surface as well as the mobility of the surface species determine the nanoparticle self-assembly, where the bulk and surface defect structure of the oxide parent is strongly entangled with the dynamics of nanoparticle nucleation and growth. In order to preserve a large nanoparticle density and fine particle dispersion over the operation time of solid oxide cells at elevated temperatures, coarsening of the nanoparticles at the oxide surface needs to be minimized, which requires the control of the oxides' defect chemistry.

In the present study, we demonstrate fundamental differences in the exsolution behavior of nickel dopants in strontium titanate host lattices with *n*-type and *p*-type character. For this purpose, we control the defect chemistry of the perovskite parent oxides by chemical (co)-doping and synthesize atomically smooth epitaxial thin films of the materials by pulsed laser deposition. The thin films are employed as well-defined model systems to study the material response in annealing experiments.

The nucleation and self-assembly of metal nanoparticles at the perovskite surface is investigated with respect to the mass transfer kinetics and thermal stability. A multi-method approach of oxygen tracer exchange studies, *ex-situ* morphological investigations, high-resolution transmission electron microscopy of the catalysts surface region and *in-situ* ambient pressure x-ray photoelectron spectroscopy reveals a considerable impact of the chemical doping strategy on the exsolution behavior. We show that the type and concentration of defects at the metal-oxide interface can strongly influence the thermal stability of exsolved metal nanoparticles. Strikingly, a high thermal stability of nanoparticles at the surface of the investigated *n*-type perovskite is not related to anchoring of the nanoparticles at the oxide support, but related to the surface defect chemistry, which can be tailored by surface engineering using oxide epitaxy.

## Photoluminescence analysis of 2D nanolayers synthesized by CVD method

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Keywords: MoS<sub>2</sub>, TMDC, epitaxial growth, CVD, Photoluminescence

Contribution: Poster

We report about the photoluminescence characterization of TMDCs layers (MoS<sub>2</sub> and WS<sub>2</sub>) synthesized by Chemical Vapor Deposition technique. Thermally annealed and UV- Ozone treated c-plane oriented sapphire substrates were used to stimulate epitaxial growth of highly aligned molybdenum disulfide and tungsten disulfide samples. The performed AFM analysis, photoluminescence and Raman spectroscopy reveals the synthesis of nanoclusters with a triangular shape and lateral dimensions of 5-10 microns and a cluster height of approximately 1 nanometer, confirming monolayer formation. Assembling of heterostructures for solar cells

applications will be presented and discussed.

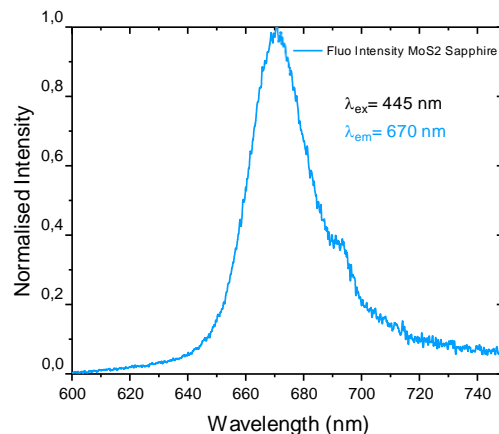
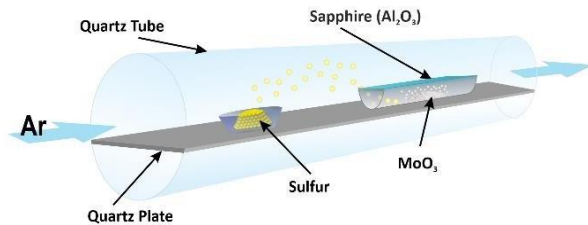


Figure 1. Experimental CVD set-up and photoluminescence spectra of MoS<sub>2</sub> under 445 nm excitation.

Reference:

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**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”



## Electric-field engineered lattice distortions for optoelectronic devices

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Keywords: strain-engineering, orbital-ordering, optoelectronics

Contribution: Oral

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  $\text{RNiO}_3$ ,  $\text{AFeO}_3$  and  $\text{RMnO}_3$  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 unprecedented 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 assemble 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  $\text{ABO}_3$  families with  $e_g^1$  occupation of the B-site  $d$ -orbitals, such as the 3-3 rare-earth manganites ( $\text{RMnO}_3$ ) that present Jahn-Teller effect. DFT calculations predict that this polar phase can be strain-engineered in a few perovskites, such as  $\text{YMnO}_3$ ,  $\text{SrTiO}_3$ ,  $\text{BaMnO}_3$  and  $\text{BiFeO}_3$  [1]. We chose  $\text{SrTiO}_3$  and  $\text{YMnO}_3$ , 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  $\text{YMnO}_3$  and  $\text{SrTiO}_3$  between 1.8 and 3 eV. For this, we used PLD to deposit epitaxial  $\text{YMnO}_3$  and  $\text{SrTiO}_3$  thin-films onto  $\text{LaMnO}_3$  and  $\text{MgO}$  buffer layers deposited in Si, to reach a tensile strain between 3 and 5%, to stabilize the polar  $\text{Pb}_{21m}$  phase. This  $\text{Pb}_{21m}$  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  $\text{Pb}_{21m}$  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.

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## Electrical characterisation and nanomanipulation of $\text{MoO}_{3-x}$ monolayer grown on graphite

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Paweł Dąbrowski<sup>1</sup>, Maxime Le Ster<sup>1</sup>, Witold Kozłowski<sup>1</sup>, Rafał Dunał<sup>1</sup>,  
Przemysław Przybysz<sup>1</sup>, Wojciech Ryś<sup>1</sup>, Klaudia Toczek<sup>1</sup>, Paweł J. Kowalczyk<sup>1</sup>, Maciej Rogala<sup>1</sup>

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Keywords: epitaxial molybdenum trioxide; van der Waals structure; conductive atomic force microscopy; nanomanipulation

Contribution: Oral

Abstract:

Orthorhombic molybdenum oxide has many unique properties, such as a wide band gap (about 3.2 eV) and a high relative permittivity. Additionally, ultrathin layers of this material are transparent and have good mechanical properties, making them an excellent candidate for use in stretchable and flexible electronics and optoelectronics applications. Particularly interesting are the monolayers of  $\text{MoO}_3$ , which have great potential to be used to alter the properties of graphene electrodes in optoelectronic devices.

Monolayers of molybdenum oxide were deposited under ultra-high vacuum conditions by thermal evaporation from the Knudsen cell. The layer was grown on highly orientated pyrolytic graphite (HOPG), which, as a conductive substrate, enables precise, nanoscale electrical characterisation using a conductive atomic force microscope (c-AFM) probe.

We present AFM investigations on an epitaxially grown  $\text{MoO}_{3-x}$  layer on a graphene-like substrate, such as HOPG. Chemical composition was studied by X-ray photoelectron spectroscopy. Atomic force microscopy (semi-contact and contact mode), Kelvin probe force microscopy, and lateral force microscopy were used for nanoscale characterisation. We show movement of the unpinning island under slight mechanical stress, as well as shaping of the material with applied electrical stimulation. We show the heterogeneity of the  $\text{MoO}_{3-x}$  monolayer in terms of electrical properties.

### Acknowledgments

This work was supported by National Science Center, Poland, under the Grant 2020/38/E/ST3/00293.

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## **Epitaxial $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ thin films on vicinal $\text{SrTiO}_3$ substrates for sensitive anisotropic magnetoresistive sensors operated at room temperature**

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Keywords: vicinal substrates, uniaxial magnetic anisotropy, pulsed laser deposition, magnetic sensors, functional oxides

Contribution: Oral

The detectivity of a magnetic sensor is defined as the ratio of its intrinsic noise to its sensitivity. We previously demonstrated that very low levels of low frequency noise can be achieved in high epitaxial quality  $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$  (LSMO) thin films. Since LSMO is a room temperature ferromagnetic metal with Curie temperature around 360K, it is a good candidate for the realization of anisotropic magnetoresistive sensors operated at room temperature, even if they do not reach same sensitivity values as other spintronic sensors such as Giant Magnetoresistances (GMR) or Tunnel Magnetoresistances (TMR). Anisotropic Magnetoresistance (AMR) depends on the angle between the direction of the electrical current and that of the magnetization. It is therefore important to control the magnetic anisotropy in LSMO thin films, and in particular to achieve an uniaxial magnetic anisotropy, with a relatively low anisotropy field, named  $H_a$ , while keeping a very low electrical noise. We will present results obtained with AMR sensors patterned in 30 to 60 nm thick epitaxial  $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$  (LSMO) thin films, deposited on 4°, 6° or 8° vicinal  $\text{SrTiO}_3$  (STO) substrates by pulsed laser deposition. The use of a vicinal substrate, which presents a surface miscut angle regarding to the crystallographic plane, was used to induce uniaxial anisotropy with an easy magnetic axis along the step edge directions [1]. A Wheatstone bridge design was used in order to get rid of common perturbations, such as temperature drift. The measured AMR curves could be compared to the expected behaviour considering the Stoner-Wohlfarth model for coherent magnetization reversal.

In order to achieve a higher sensitivity, thus the targeted lower detectivity, several parameters were considered, such as LSMO film thickness, LSMO deposition temperature, vicinal angle of the substrates and design of the electrical contacts. Dedicated electronics readout and gradiometric configuration were considered. The lowest detectivity at 310K was  $1 \text{ nT}\cdot\text{Hz}^{-1/2}$  at 1 Hz and  $200 \text{ pT}\cdot\text{Hz}^{-1/2}$  at 1 kHz in a single-layer sensor without using any performance enhancing techniques such as magnetic flux focusers or modulation techniques [2]. Such AMR sensors are promising for biomedical applications where small size devices are needed at low frequency.

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## Fabrication of LaMnO<sub>3</sub> based epitaxial thin films and DFT calculation

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spintronic, epitaxial films, DFT calculations Contribution: Oral

### Abstract:

Materials based on lanthanum-manganite are catching a lot of attention from science community due to their exceptional magnetoelectric properties, such as giant magnetoresistance (GMR). A new concept of electronics, called spintronic is developed based on phenomena of GMR. In contrast to conventional electronics where charge still dominates, spintronic is based on spin properties of electron and associated magnetic moments. Due to the existence of GMR, pure and doped lanthanum manganite based materials are considered as good candidates for the application in the field of spintronic devices such as new type of magnetic memories. Beside GMR properties, materials based on lanthanum-manganite are very sensitive to external stimuli and very suitable for manipulating the structure and properties by adding dopants as Sr<sup>2+</sup>, Ca<sup>2+</sup>, etc. Specific application dictated the development of LaMnO<sub>3</sub> based material in epitaxial thin film form. Expensive physical vapor deposition methods with complex setup were reserved for the fabrication of homogenous epitaxial oxide films. In recent years, with appearance of polymer-assisted deposition (PAD), chemical solution deposition methods have found their place in the fabrication of epitaxial layers.

The aim of this research was obtaining epitaxial LaMnO<sub>3</sub> (LMO) and La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> (x=0.1, 0.3 and 0.5) thin films by polymer assisted deposition technique (PAD). LaMnO<sub>3</sub> solutions were prepared by dissolving of La(NO<sub>3</sub>)<sub>3</sub>·6H<sub>2</sub>O and Mn(NO<sub>3</sub>)<sub>2</sub>·4H<sub>2</sub>O in the distilled water, with addition of the water soluble polymers polyethyleneimine (PEI) and ethylenediamine tetraacetic acid (EDTA) in order to stabilize solution. Strontium nitrate was used as a source of Sr<sup>2+</sup> ions. Prepared pure LMO solutions were deposited by spin coating method on the previously cleaned monocrystalline SrTiO<sub>3</sub> (110 and 001) substrates and thermally treated at the 750 °C. In the next step, prepared LMO thin films were post-annealed at the temperatures up to 900 °C. Post-annealing treatment shows changes in thin films structure and helps to establish optimal temperature regime in order to obtain different LaMnO<sub>3</sub> phases. According to previous results, La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> solutions were spin coated on the SrTiO<sub>3</sub> (001) substrate and thermally treated in the same way as the pure LaMnO<sub>3</sub>. Influence of post-annealing treatment on the structure were examined, as well as magnetic behavior of thin films.

Second part of this research was application of DFT calculation to pure and Sr doped LMO systems. The ground state structure of LMO was obtained after the geometric optimization and it was used for further calculations such as band structure, total and partial density of state and electronic density difference. The obtained results were compared to experimentally obtained data and literature values.

## Tuning of the Oxidation State of Vanadium Oxide by Pulsed Laser Deposition:

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Keywords: oxidation state, pulsed laser deposition, vanadium oxide.

Contribution: Oral

Vanadium oxide compounds attracted much attention because of their unique properties and possible applications in different fields, such as charge storage/ electrochromic devices, broadband photodetectors, sensors, and others [1]. For instance, vanadium dioxide ( $\text{VO}_2$ ) undergoes a MIT transition near the room temperatures (e.g. around of 340 K) and attracted a lot of attention for thermochromic smart windows, field-effect transistors, frequency tuning devices, electronic and resistive switches or nanometer scale plasmonic devices. On the other hand, vanadium pentoxide ( $\text{V}_2\text{O}_5$ ) is a compound with reversible lithium-ion insertion/extraction processes, due to its layered structure, being a good candidate for electrochromic and charge storage applications [2]. However, due to the multivalent nature of vanadium and the lack of a good understanding of the growth control of the oxidation state, stabilization of phase pure vanadium oxides with a single oxidation state is still challenging. For this purpose, pulsed laser deposition proved its ability to obtain different stable compounds by controlling the growth conditions via the substrate temperature and oxygen partial pressure  $P(\text{O}_2)$  [3].

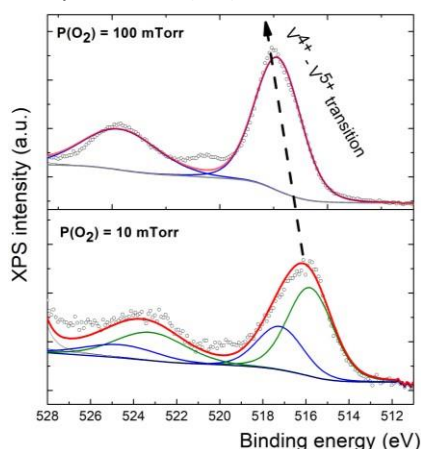


Figure 1 XPS spectra for samples obtained at low and high oxygen pressure

Herein, we have synthesized  $\text{VO}_2$  and  $\text{V}_2\text{O}_5$  compounds by pulsed laser deposition (PLD), at low and high oxygen pressure, using a one-step process, without any post-annealing processes. Furthermore, the ability of  $\text{V}_2\text{O}_5$  to be used as electrode for charge storage devices is shown by specific electrochemical measurements.

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### Acknowledgments

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## Unveiling the potential of spray-coated Pr:SnS<sub>2</sub> thin films for photocatalytic and antibacterial applications

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Keywords: Tin sulfide; SnS<sub>2</sub>; Pr-doped SnS<sub>2</sub>; Photocatalysis; Photocatalysts; Antibacterial studies

Contribution: Poster

Abstract:

Pristine and Praseodymium (Pr)-doped tin sulphide (SnS<sub>2</sub>) thin films were successfully fabricated using an eco-friendly spray-coated approach. This study presents a comprehensive analysis of the structural, morphological, chemical, photocatalytic, and antibacterial properties of the fabricated films. The pristine and Pr-doped SnS<sub>2</sub> thin films exhibited a hexagonal crystal structure with a preferential growth along the (1 0 1) plane. As the Pr-doping increased, an increase in crystallite size was observed. The Raman spectra analysis identified a characteristic band at 315 cm<sup>-1</sup>, assigned to the A<sub>1g</sub> mode, representing the vibrations of Sn-S along the c-axis of the cell structure. X-ray photoelectron spectroscopy (XPS) confirmed the presence of Sn, S, and Pr in the synthesized thin films, consistent with the experimental values of undoped and Pr-doped SnS<sub>2-x</sub> composition. Additionally, XPS analysis revealed the presence of Pr<sup>3+</sup> oxidation state in the Pr-doped SnS<sub>2</sub> films. The photocatalytic degradation potential of the Pr-doped SnS<sub>2</sub> thin films against Congo Red improved with increasing percentage of Pr<sup>3+</sup> doping. Moreover, the antibacterial activity against Escherichia coli bacteria was enhanced with higher Pr-doping content. This study introduces a novel and simple approach utilizing Pr-doped SnS<sub>2</sub> thin films for photocatalytic degradation of organic pollutants and mitigation of microbial growth.

**APPLICATION OF NANOPOROUS ANODIC ALUMINIUM OXIDE MEMBRANES IN VARIOUS INDUSTRIES OR  
FIELDS**

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**Keywords:** nanopores, membranes, Anodic Aluminium Oxide, anodization

Contribution: Poster

**Abstract**

Nanoporous membranes, which have small pores or openings at the nanoscale, have unique properties that make them valuable in a wide range of industries. These membranes find application in industries such as water treatment, pharmaceuticals, food and beverage, biotechnology, energy, and many others. They are utilized for tasks such as filtration, separation, purification, controlled release, and sensing, among others. The versatility and adaptability of nanoporous membranes make them suitable for diverse industrial applications, offering enhanced efficiency, selectivity, and performance in specific processes or systems.

One of the promising materials for creating nanoscale membranes is nanoporous anodic aluminum oxide (AAO, alumina) [1]. This material has a precise, self-assembled honeycomb structure composed of parallel nanopores with no lateral crossovers between individual pores. AAO can be easily fabricated by simple anodization of aluminum in an acidic electrolyte. Different anodization regimes can be applied in the fabrication process, leading to different pore diameters in the range of 10-450 nm. AAO is a very suitable template for immobilization of the biological molecules, due to the adjustable pore size and interpore distance. Furthermore, nanoporous AAO is optically transparent, electrically insulating, chemically stable, bioinert, and biocompatible. These outstanding properties are beneficial for various applications of AAO membranes in biotechnology and medicine ranging from biofiltration membranes, lipid bilayer support structures, biosensing devices, and implant coatings to drug delivery systems with AAO capsules and scaffolds for tissue engineering. Furthermore, AAO also serves as a widely used template for other biocompatible nanostructures such as gold and platinum nanopillars. For that reason over the past years, the development of novel biomedical applications has benefited immensely from the unique properties of AAO membranes. Despite the proven utility of those nanofabrication methods, there is still a lack of simpler and cheaper procedures to expand the usage of this nanotemplate.

High-quality AAO (anodic aluminum oxide) films provide ordered straight channels, with a diameter of 10–500 nm, pore density of  $10^7$ – $10^{11}$  pore/cm<sup>2</sup>, and thickness of 1–300 μm [1,2]. With large surface areas, high mechanical strength, and flexibility, AAO can be used in medical or energy applications, such as drug delivery and detection. The large AAO surfaces can be utilized to absorb the bio-indicators or drugs, and the releasing behavior can also be controlled based on the heat sensitivity. AAO has also found applications in energy conversion between carbon dioxide (CO<sub>2</sub>) and methanol (CH<sub>4</sub>) [4]. By loading photocatalyst particles on the AAO surface, such photocatalytic systems can be used to recycle carbon dioxide into organic compounds. Based on the features of larger surface areas and nanochannels for mass delivery and gas diffusion, three-dimensional (3D) structure of AAO films have practical advantages over two-dimensional (2D) AAO films for medical and energy applications.

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## **Unlocking Innovation Through Application-Oriented Material Development**

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Keywords: Application-oriented Material Development, Innovation and Commercialization

Contribution: Poster

### Abstract

Application-oriented material development, a catalyst for scientific innovation, is key across various sectors. This article emphasizes the importance of attending a dedicated academic conference on this topic. Through exploring latest trends and challenges, we reveal the transformative potential of these purpose-built materials. Exceptional properties enable breakthroughs in electronics, healthcare, energy, and transportation, revolutionizing how we live. The conference allows exposure to cutting-edge research, equipping attendees with knowledge to innovate in their work. Overcoming challenges related to material selection, synthesis, scalability, and performance optimization is crucial. The conference encourages sharing experiences, fostering collaborations, and finding innovative solutions. As a networking platform, it facilitates connections among researchers, industry leaders, and policymakers, promoting interdisciplinary research, technology transfer, and commercialization. The development of these materials has implications for energy systems, healthcare, environmental protection, transportation, and infrastructure, enhancing societal well-being. Attending such a conference is an opportunity to broaden knowledge, foster collaborations, and contribute to this transformative journey, thereby driving innovation and shaping a brighter future for industries and society.



## Investigating the effect of thermal annealing and changing the concentration of GO in GO/PVA nanocomposites on their structural, electrical, and optical properties

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**Keywords:** GO/PVA nanocomposites; the influence of thermal annealing; concentration; physical properties; band gap value

**Contribution:** Poster

The combination of PVA and GO can function as an alternate electrode in supercapacitors and lithium-ion batteries due to its outstanding electrical characteristics. It is important to study the temperature and concentration dependence of the properties of devices and elements based on GO/PVA. The results of this research will allow for optimizing the parameters of devices and elements to be created based on these composites. At the same time, determining temperature-resistant materials by testing sample thermal stability and their use in relevant fields are critical challenges.

The GO was synthesized by the modified Hummers method. GO/PVA nanomaterials have been prepared in different amounts of GO (1, 2, 3, 5, and 20%). To investigate the effect of temperature on the physical properties of GO/PVA composites prepared at different percentages, they were thermally annealed at different temperatures (40°C, 70°C, and 110°C). The crystallite size of the 2% GO/PVA composite was determined depending on the temperature and the percentage of GO in the PVA matrix. In order to determine the effect of thermal annealing temperature on the optical properties of GO/PVA composite, band gap values were calculated on the example of 2% GO/PVA composite. The variation of the band gap value for GO/PVA composites with 2% concentration depending on the thermal annealing is shown in Table 2.

**Table 1.** Dependence of the band gap on thermal annealing for 2% concentrated GO/ PVA composite

Composite	25 °C	40 °C	70 °C	110 °C
2% GO / PVA	2.40 eV	2.35 eV	2.30 eV	2.20 eV

As can be seen in Table 1, the band gap value decreases with the increase in the temperature of the thermal annealing. The reason for this is that the mobility of the polymer increases with the increase in the temperature of the thermal annealing, and their aggregation processes become easier. As a result, the size of the particles increases. This leads to a decrease in the band gap value.

Dependence of the specific resistance of 1% (a), 2%(b), 3% (c), 5%(d), and 20% (e) concentrated GO/PVA composite on the logarithmic value of electric field frequency at different temperatures.

Based on the results obtained from the study of the electrical properties of the samples, it can be summarised that annealing at elevated temperatures can facilitate the reduction of functional groups of GO, resulting in increased electrical conductivity and a decrease in specific resistance. At the same time, the influence of the temperature as a result of the structural reorganization within the GO/PVA composite can lead to better alignment and connectivity of the GO sheets, which improves charge transport pathways and reduces resistance. As a result of the reduction of defects enhances charge carrier mobility and conductivity, resulting in a decrease in specific resistance.

## Preparation of DAOx immobilized AuNPs@CQD for optical sensor applications

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Keywords: DAOx, AuNPs, optical sensor, CQD  
Contribution: Poster

### Abstract

The immobilization of enzymes on nanomaterials has become interesting in order to increase their stability in recent years. In present study, diamine oxidase (DAOx) was immobilized on gold@carbon quantum dots (AuNPs@CQD) for optical sensor application. CQD was synthesized by electrochemical method using carbon sources such as carbon nanotube and graphite as starting material and/or by hydrothermal method using carbon sources such as citric acid and glucose as starting material. AuNPs was synthesized in quantum dots solution by adding H<sub>2</sub>AuCl<sub>4</sub>. The solution mixture was stirred for a certain time at 100 °C until a stable purple color was obtained. AuNPs@CQD was characterized by X-ray photoelectron spectra (XPS) and Fourier transform infrared spectroscopy (FTIR). Then DAOx was immobilized on AuNPs@CQD by electrostatic interaction and crosslinked. Glutaraldehyde was used as a crosslinker. The stability and activity of DAOx immobilized AuNPs@CQD were determined using putrescine and histamine as substrates and compared with free enzyme solution.

## Synthesis and Characterizations of Perovskite Quantum Dots and Carbon Quantum Dots as Core Shell Structure

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Keywords: Perovskite, Quantum Dot, Core Shell, Synthesis, Characterization

Contribution: Poster

### Abstract:

Perovskite nanocrystals have shown great potential for use in optoelectronic devices in recent years. Due to their superior photoluminescence quantum efficiency (PLQY), tunable emission wavelength, and low-cost simple synthesis protocols [1]. Despite the apparent exceptional benefits, the environmental stability of lead halide perovskite nanocrystals remains a major challenge that significantly obstructs their practical applications and scalability for commercialization. Core/shell metal halide nanocrystal technology has played an important role not only in improving luminescent properties, reducing exciton recombination, suppressing non-radiative recombination, and improving charge carrier transport, but also improving the performance of semiconductor materials as well as environmental stability. It is thought that core shell structures can improve the operational stability and performance of devices by providing a solution to the stability problem. Traditionally, core/shell NCs are commonly engineered by a two-step procedure: first the synthesis and purification of the core, followed by the overgrowing of a shell at different reaction temperatures. The strategies for the synthesis of perovskite core/shell nanostructures were quite dissimilar to conventional methods due to the inherent soft ionic nature of the perovskite lattice, low melting points, high ion mobility, and fast reaction rates. In this study, the core shell structure was synthesized using the hot injection method. Optical and morphological characterizations of the synthesized core shell structures were made.

### Acknowledgements

The authors thank to financial support of the Scientific and Technological Research Council of Turkey (TÜBİTAK) (PN:121F377)

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## Synthesis of Perovskite Quantum Dots and Their Using in Perovskite SolarCells as Additive

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Keywords: Perovskite, Solar Cell, Quantum Dot, Perovskite Quantum Dots, Synthesis, Characterization

Contribution: Poster

### Abstract:

Lead halide-based perovskite quantum dots (PQDs), which is the rising trend of recent years, has emerged as an important material class for optoelectronic and photo electrochemical applications. These structures, which have become popular due to their quantum confinement effect and defect- resistance, have tunable band gaps, tunable wavelength that covers the entire visible spectrum, narrow emission spectrum, high charge carrier mobility, remarkable light absorption, compatibility with flexible/stretchable electronics, high photoluminescence quantum efficiency and interesting features such as long charge diffusion length allow them to be used in many fields [1, 2]. In the study, the synthesis of perovskite quantum dots, LARP (ligand-assisted re-precipitation) method was used. In this method, PQDs were synthesized in suitable amounts of  $PbX_2$  and  $Cs_2CO_3$  in oleylamine, octadecene and oleic acid at room temperature with the help of an ultrasonic rod for 30 minutes by vigorous stirring and separated from their solvent by centrifugation. The optical analyzes of the synthesized PQDs were characterized by UV–Vis and photoluminescence spectrometry, and their structural and morphological characterizations were characterized by XRD, SEM and TEM techniques. Synthesized PQDs have been used as additive in perovskite solar cells to improve their charge-carrying properties and thus their performance. For this purpose, PQDs were added to the perovskite solution to increase the energy conversion efficiency of perovskite solar cells with ITO/PEDOT:PSS/Perovskite:PQDs/PCBM/BCP/Ag arrays. Thin films and solar cells have been characterized by appropriate techniques to elucidate the effect of PQDs on their structural, optical and surface properties.

### Acknowledgements

The authors thank to financial support of the Scientific and Technological Research Council of Turkey (TÜBİTAK) (PN:121F377)

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## Magnetocaloric and Giant Magnetoresistance Effects in La-Ba-Mn-Ti-O Epitaxial Thin Films

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Keywords: Epitaxial thin films, perovskite manganite, magnetoresistance, magnetocaloric effect;

Contribution: Poster

Abstract:

Magnetic perovskite films have promising properties for use in energy-efficient spintronic devices and magnetic refrigeration. Here, an epitaxial ferromagnetic  $\text{La}_{0.67}\text{Ba}_{0.33}\text{Mn}_{0.95}\text{Ti}_{0.05}\text{O}_3$  (LBMTO-5) thin film was grown on  $\text{SrTiO}_3(001)$  single crystal substrate by pulsed laser deposition. High-resolution X-ray diffraction proved the high crystallinity of the film with tetragonal symmetry.

The LBMTO-5 epilayer exhibits a second-order ferromagnetic-paramagnetic phase transition around 234 K together with a metal–semiconductor transition close to this Curie temperature ( $T_c$ ). An in-plane uniaxial magnetic anisotropy was evidenced. The magnetic entropy variation under 5 T induction of a magnetic field applied parallel to the film surface reaches a maximum of  $17.27 \text{ mJ/cm}^3 \text{ K}$ . The relative cooling power is  $1400 \text{ mJ/cm}^3 \text{ K}$  (53% of the reference value reported for bulk Gd) for the same applied magnetic field. Giant magnetoresistance of about 82% under 5 T is obtained at a temperature close to  $T_c$ .

## PLD growth of strontium titanate thin films on silicon substrate for photoelectrochemical water-splitting

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Keywords: **pulsed laser deposition, epitaxy, strontium titanate, thin film, rGO buffer layer, photo-electrochemistry**

Contribution: **Poster**

Abstract

Epitaxial films of metal oxides deposited on silicon substrates represent a new type of material that could be used as protective (or electroactive) layer in the photoelectrochemical water splitting. To understand the influence of crystalline and interfacial properties of oxide layer on the water splitting process a ~10 nm strontium titanate (STO) films have been grown using the PLD method on bare and reduced graphene oxide (rGO) buffered silicon substrate. Our approach relied on the oxide-silicon integration using combination of SrO-assisted deoxidation and controllable coverage of silicon surface with a mono- to three-layer of spin-coated GO. The STO films have been grown at 515 and 700 °C and various experimental techniques were used to examine the surface and crystalline properties of grown films (reflection high energy electron diffraction, atomic force microscopy, scanning electron microscopy, X-ray diffraction, X-ray reflectivity and X-ray photoelectron spectroscopy). The results show that the best the crystallinity of the STO thin films was obtained on rGO/SrO deoxidized silicon surface at 515 °C. Future studies will be devoted to electrochemical characterization of the grown films, that will help to establish clearer link on how the interface and crystalline parameters affect the water splitting process.

## Development of GaAsBi MQWs technology for NIR emitters

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Keywords: GaAsBi, laser diodes, quantum wells, MBE, photoluminescence.

Contribution: Poster

Laser diodes are the most popular type of laser devices. Although this area is well developed, there is still a need for a various set of parameters containing laser diode (LDs) operating in the near-infrared (NIR) region. Bismides, namely, GaAsBi are a group of promising compounds due to the large band gap reduction. The replacement of arsenic atoms by bismuth in GaAs lattice results in  $E_g$  reduction of up to 90 meV for 1% of bismuth in GaAsBi. The incorporation of around 6% of Bi into GaAsBi multiple quantum wells allows the fabrication of laser diodes operating in  $1 \mu\text{m} \div 1,3 \mu\text{m}$  wavelength spectral region [1]. Such LDs could be used in detection systems for exciting gases such as CO<sub>2</sub>, CO or CH<sub>4</sub>. Furthermore, GaAsBi MQW based laser diodes have showcased good performance in RT, mitigating the need for cooling [2]. Additionally, only a small concentration of Bi is necessary for a large reduction of band gap, which is useful in maintaining good strain balance. All these reasons make GaAsBi devices more attractive in comparison to the already well developed InGaAs technology.

This work focuses on optimization of the growth technology of GaAsBi multiple rectangular quantum wells (MRQWs) using GaAs barriers, to achieve the desired emission wavelength and sufficient PL intensities. The structures were grown using a molecular beam epitaxy system (Veeco GENxplor R&D). Photoluminescence measurements were performed to determine the influence of bismuth flux, arsenic to gallium ratio and the substrate temperature on the intensity and emission wavelength. X-Ray diffraction and AFM were used to investigate the composition, quality of the samples and the sharpness of the interfaces.

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## Investigation of the AlN Buffer Layer Role in Optimizing the AlGaN/GaN Nonlinear Optical Waveguide Structure

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Keywords: Nitrides, waveguides, MOCVD, buffer layer, AlN, GaN, AlGaN, SHG.

Contribution: Poster

This work explores the influence of the AlN buffer layer to the growth and properties of AlGaN/GaN nonlinear optical waveguides. GaN is a well-known material in the industry as an LED of UV spectral range. However, it can be utilized as a passive optical component – a waveguide. GaN is a non-linear crystal with non-zero second order nonlinearity parameter, hence its' ability to generate second harmonic. This exceptional feature is successfully utilized in the manufacture of second harmonic generating waveguides, which can be applied in integrated photonic-electronic circuits.

Metalorganic chemical vapor deposition (MOCVD) was chosen as a method of waveguide growth. Trimethylgallium (TMGa), trimethylaluminum (TMAI), and ammonia (NH<sub>3</sub>) were used as precursor materials during growth. AlN buffer layer were divided into three groups and were grown by changing the main growth parameters in each group. In the first group, the influence of annealing duration was investigated, in the second – sapphire nitridation and AlN nucleation temperature, and in the third – AlN nucleation duration. Every sample was characterized via atomic force microscopy (AFM), x-ray diffraction (XRD), and scanning electron microscopy (SEM). After AlN layer characterization, AlGaN/GaN waveguides structures were grown on top. Final GaN waveguide surface morphology was investigated via AFM. Optimal AlN buffer layer growth conditions were determined according to the best surface roughness of the final GaN waveguide, and AlN dislocation densities provided by XRD rocking curves.

The best recorded GaN RMS surface roughness was 3.171 nm. The latter structure was grown atop of unannealed AlN buffer layer grown for 315 s at 645 °C, on top of sapphire substrate nitridated for 200 s at 645 °C. Latter AlN buffer layer exhibited screw dislocation density of  $2.09 \cdot 10^8 \text{ cm}^{-2}$ , and mixed dislocation density of  $1.51 \cdot 10^{10} \text{ cm}^{-2}$ .



Figure 1. MOCVD grown AlGaN/GaN waveguide structure.



## Artificial Synapses made of ferroelectric epitaxial $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{O}_2$ / $\text{SrTiO}_{3-\delta}$ on silicon

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Contribution: Oral

Abstract:

Hafnia-based ferroelectric memristors in the FTJ configuration are good candidates for low power in-memory and bio-inspired neuromorphic computing [1]. Scaling of HZO below 5 nm is difficult [2] so double layer HZO/Al<sub>2</sub>O<sub>3</sub> FTJ are used [3] which however suffer from high voltage operation and significant retention loss.

Here, we report on single layer FTJ-type of devices with 5 nm HZO and 10-20 nm thick SrTiO<sub>3-δ</sub> semiconductor bottom electrode directly integrated on Si(001) substrates by molecular beam epitaxy. HZO is grown on SrTiO<sub>3-δ</sub> with preferential in plane and out of plane orientation enforced by domain matching epitaxy [4].

Due to partial polarization, a large number of stable intermediate resistance states ( $\geq 16$  states – 4 bit memory) have been observed with no significant retention loss. A time-voltage tradeoff has been observed that makes it possible to update the conductance weights by time-correlated identical pulses to obtain linear and symmetric synapse potentiation and depression. Pair pulse facilitation (PPF)/depression and Spike Timing Dependent plasticity (STDP) are also observed in  $\sim$  ms,  $\mu$ s and 100 ns time scales using record low voltages in the 1V-2V range, compatible with CMOS voltage scaling. Ionic contributions due to redox processes have a beneficial effect on the synaptic behavior, increasing the dynamic range at timescales longer than a few tens of  $\mu$ s. In addition, the ionic motion has a signature in the retention since it causes a drift of the high resistance state to higher resistance values. This increases the memory window thus improving reliability.

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## Epitaxial stabilization of ferroelectric HfO<sub>2</sub> via doping and interface effects

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Keywords: Ferroelectric oxides; HfO<sub>2</sub>; Epitaxial stabilization; Epitaxial stress engineering; High lattice mismatch

Contribution: Oral

The robust ferroelectricity of a metastable orthorhombic phase of doped-HfO<sub>2</sub>, a CMOS compatible material, makes this oxide extremely promising for memory devices. Epitaxial stabilization of this high-energy phase is challenging, [1] and achieving single-phase epitaxial films has been elusive for many years. Here we show that domain matching epitaxy allows for the stabilization of the ferroelectric phase in doped HfO<sub>2</sub> films on perovskite single crystals despite the enormous structural differences. We have found that the ratio of interface energy of competing polymorphs with the bottom electrode depends on the epitaxial stress, and this allows tailoring of the ferroelectric phase content by substrate selection. The particular dopant atom and its content is another critical factor in stabilizing the ferroelectric phase. Interestingly, chemical doping and epitaxial stress do not compete and can be both used to synergistically tailor ferroelectric properties. The relative content of ferroelectric and paraelectric phases, adjusted by suitable selection of substrate and HfO<sub>2</sub> doping, allows control of ferroelectric polarization, endurance and switching time.

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## Improving the Properties of Superconductor/Ferromagnet Heterostructures

### $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}/\text{CaRuO}_3$

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Keywords: Pulsed Laser Deposition, superconductivity, ferromagnetism, heterostructures

Contribution: Poster

Abstract:

Superconductor/ferromagnet heterostructures are of great interest because of the wide range of applications where they can be used, such as superconducting electronics.  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$  (YBCO), with a critical temperature of around 90 K, is one of the most studied superconductors, also in the form of YBCO/ferromagnet heterostructures. The properties of the thin films are highly dependent on the quality of the films, which can be tuned by the deposition conditions and deposition order of the layers. We used by Pulsed Laser Deposition to obtain YBCO and  $\text{CaRuO}_3$  thin films with the layers either in direct contact or separated by a 5 nm  $\text{SrTiO}_3$  layer [1] and investigated the impact of a ferromagnetic layer on the properties of YBCO using extensive measurements of the magnetic moment of the superconductor and ferromagnet as a function of magnetic field and temperature. Then, the deposition order of the layers was changed and it was shown that both the superconductivity of YBCO and the ferromagnetic properties of CRO are influenced by the deposition order and thickness of the films. XRD analysis was performed to correlate the physical properties mentioned above with the materials' structure.

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## Controlling the quality of thin film multilayers in large area wafers for industry-relevant sensor applications

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Keywords: spintronics, magnetic sensors, thermal stability, thin films Contribution: Oral

### Abstract

Magnetic field sensors have a mature and transversal level of implementation in the market, from automotive to biomedical domains. The impressive technological progress in thin film preparation and characterization, combined with nano-microfabrication tools offer presently large spectra for device design. The materials discussed include several varieties of thin film materials combined onto multilayer stacks, where the quality of the ultrathin layers and interfaces are crucial for the final magnetic and electrical performance. Examples where spintronic sensors are useful tools for precision sensing will be provided, including integration with microfluidics. In this talk, I will show how challenging applications have triggered creative solutions, requiring joint skills in transversal areas as physics, materials and microelectronics engineering.

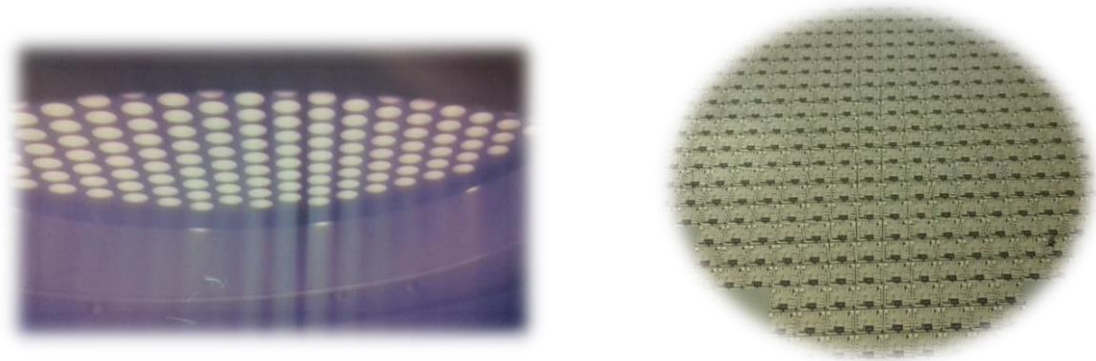


Figure 1- (left) Broad beam deposition detail of the grids for ion extraction. (right) Spintronic sensors microfabricated on a 200mm diameter wafer.

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## **Optimization of Epitaxy Conditions of InGaAs and GaAsBi Multiple Quantum Well Structures for Applications in NIR VECSELS**

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Keywords: multiple quantum wells, molecular beam epitaxy, photoluminescence mapping, vertical- external-cavity surface-emitting laser, near infrared.

Contribution: Oral

Microlaser is the core component of various sensing systems applied in many fields, such as Raman spectroscopy and material processing, LiDAR and transport traffic systems, food analysis and ambient pollution monitoring, medical diagnostics. The main parameters that define the priorities of lasers applications are emission wavelength, beam quality, wavelength tunability, output power and the size of the device [1, 2]. Vertical-external-cavity surface-emitting lasers (VECSEL) are a relatively new laser family that overcomes key problems typical to conventional semiconductor lasers and combines desirable properties: high optical power and circular beam quality. It is very important to understand how crystal growth influences the characteristics of a microlaser. From a technological point of view, there are numerous epitaxy limitations causing structural defects or features reducing the optical quality [3]. Thus, the optimization of the laser gain region composition and architecture becomes a crucial fundamental process.

In this work the main activity was focused to investigation of the technological parameters required to grow high quality quantum structures of two different materials, InGaAs and GaAsBi, on GaAs substrate, balance the strain between quantum well and barrier layers, obtain sharp interfaces and perform complex investigation of optical properties. The multiple quantum well structures (MQWs) were grown using solid-source Veeco GENxplor R&D MBE system equipped with standard cells for metallic In, Al, Ga, Bi and unique As design source generating arsenic dimers flux.

Photoluminescence measurements were performed to determine the influence of growth conditions, In/Ga, As<sub>2</sub>/Ga beam equivalent pressure ratios, Bi flux, growth rate and substrate temperature, on emission energy and intensity.

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## Is another epitaxial relationship of ZnO thin films on c-cut sapphire possible?

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Keywords: epitaxy, ZnO thin films

Contribution: Oral

Zinc Oxide (ZnO) thin films grow with their c-axis normal to the substrate, leading to a columnar microstructure with the (002) planes parallel to the surface substrate. The classical in-plane epitaxy of ZnO thin films on c-cut sapphire single crystal substrates presents a 30° rotation between the two hexagonal unit cells of ZnO and c-cut sapphire [1]. In this work we report on the new well-defined epitaxial relationship between the (229) ZnO on (002) sapphire plane although the large lattice and symmetry mismatch.

Nd doped ZnO thin films (Nd:ZnO) were grown by pulsed-electron beam deposition (PED) on c-cut sapphire substrates under oblique angle incidence at 10<sup>-2</sup> mbar oxygen pressure and 500°C substrate temperature. PED is a growth method similar with pulsed laser deposition that has the advantage to grow stoichiometric, homogenous, epitaxial oxide thin films with tunable physical properties at lower costs. X-ray diffraction, pole figures analyses and transmission electron microscopy were performed. The films were smooth, compact with columnar grains inclined at about 17°±4° from the normal to the substrate surface. By means of X-ray diffraction and transmission electron microscopy experiments, the würtzite phase of Nd:ZnO thin films was evidenced with the c-axis inclined around 35° with respect to the normal axis of the substrate, with a three-fold azimuthal symmetry.

Pole figures were used to determine the epitaxial relationships between Nd:ZnO thin films and sapphire substrate. The 35° angle tilt of the ZnO c-axis from the normal to the substrate was explained by the epitaxy of the (229) ZnO plane on the (002) sapphire plane. This particular orientation, that was never reported previously, is obtained from the rotation of the [001] ZnO direction around the [1-10] ZnO one, which allows the (229) ZnO plane to be parallel to the (002) sapphire substrate [1]. The unusual epitaxy will be discussed in the frame of domain matching epitaxy approach together with the effect of the specific growth on the electrical and optical properties of films. These c-axis tilted epitaxial Nd:ZnO thin films are attractive for sensitive and disposable biosensors functioning as acoustic resonators in shear mode for biological and medical applications.

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