# European Conference on Innovative and Advanced Epitaxy

## Organized by the EU COST Action OPERA

**Pisa, May 19-23, 2025**

OPERA
COST Action CA20116

Dear colleagues,

It is our great pleasure to welcome you to the **OPERA conference “European Conference on Innovative and Advanced Epitaxy”**, **Pisa/Italy**.

**This conference covers the scientific tasks of the OPERA COST Action, though the 3 WorkGroups:**

- **WorkGroup 1: Fundamental research – New Materials:** *In material science, the ambition is to address new challenges, pushing the frontiers of knowledge. To address SDGs: the fundamental key in the epitaxy field must be addressed for mastering “actual” materials and developing new materials.*
- **WorkGroup 2: Applications-oriented material developments:** *Optimization of materials for innovative devices: Novel device performances rely on material properties. In this regard, materials must be developed considering device requirements.*
- **WorkGroup 3: Industry-oriented materials development and technological transfers:** *To develop technological transfer-ready devices, the fundamental challenges of tasks 1 & 2 must be addressed by taking into account market–proof device specifications.*

**This conference aims to strengthen and promote communication and interaction between the European epitaxy community involving academic and startup/Industrial partners.**

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

All committee members are happy to meet you in Pisa.

Conference Chairs

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COST is supported by the EU Framework
Programme Horizon 2020

# European Conference on Innovative and Advanced Epitaxy

**Pisa, May 19-23, 2025**

## May 19, 2025

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|---|---|
| **13h00** | **Registration** |
| **14h00** | **Welcome** |
| **14h20** | *S1-01* - **Matthew Zervos**<br>Taking the Crystal Growth of Cu2O to a New Level"<br>*School of Engineering, University of Cyprus* |
| **14h40** | *S1-02* - **Marta Sawicka**<br>Extreme doping of GaN with Si and Ge by plasma-assisted molecular beam epitaxy<br>*Institute of High-Pressure Physics Polish Academy of Sciences, Poland* |
| **15h00** | *S1-03* - **Adina Diana**<br>Epitaxial Growth of Iron and Cobalt on Oxide Substrates<br>*National Institute of Materials Physics, Romania* |
| **15h20** | *S1-04* - **Esme Isik**<br>Novel growth method for TiN on GaAs(001) and TiO2<br>*Department of Electronics and Automation, Turkey* |
| **15h40** | *S1-05* - **Sabrina Corbellini**<br>Rotational domains in epitaxial Ga2O3: identification of their origin and new strategies to prevent them<br>*University of Parma, Italy* |
| **16h00** | **Coffee Break** |
| **16h40** | *S2-01* - **Fatih Akyol**<br>Optimization of Growth Parameters in the LPCVD of UWBG Rutile Germanium Dioxidel<br>*Yildiz Technical University, Turkey* |
| **17h00** | *S2-02* - **Renata Butkutė**<br>Segregation-driven formation of Bi-QDs in GaAsBi layered structures<br>*Center for Physical Sciences and Technology, Lithuania* |
| **17h20** | *S2-03* **María Ángela Pampillón**<br>GaP on Si integration by chemical beam epitaxy<br>*Universidad Autónoma de Madrid, Spain* |
| **17h40** | *S2-04* - **Merve Nur Koçak**<br>MOVPE Optimization of InGaAs/InAlAs Superlattices: Influence of $AsH_3$ Flow and Interface Transition on Structural Properties<br>*Sivas Cumhuriyet University, Turkey* |
| **18h00** | *S2-05* - **Khaoula El Mechyly**<br>Fabrication and Characterization of Germanium Nanoribbons on Aluminium (110) via Molecular Beam Epitaxy<br>*Université de Haute Alsace, Institut de Science des Matériaux de Mulhouse, France* |
| **18h20** | **Women in Science** |

## May 20, 2025

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| **8h30** | **Registration** |
| **9h00** | *S3-01* - **Andrea Zelioli**<br>Optimization of AlGaAs Barriers in InGaAs Quantum Wells for Enhanced Near-Infrared Emission<br>*State research institute Center for Physical Sciences and Technology, Lithuania* |
| **9h20** | *S3-02* - **Abderrahim Moumen**<br>Epitaxial Growth of ▯ and ▯ $Ga_2O_3$ Polymorphs for Efficient Self-Powered p-n Photodiodes<br>*University of Parma, Italy* |
| **9h40** | *S3-03* - **Giovanni Isella**<br>Heteroepitaxial microcrystals for infrared photonics integration<br>*Politecnico di Milano, Italy* |
| **10h00** | *S3.04* - **Emmanouil Dimakis - *Invited Speaker***<br>Challenges in the epitaxy of three-dimensional heterostructures: the case of lattice-mismatched core/shell nanowires<br>*Helmholtz-Zentrum Dresden-Rossendorf, Germany* |
| **10h40** | **Coffee Break** |
| **11h20** | *S4-01* - **Stavros Panos**<br>TiN Nanotriangle Fabrication via Nanosphere Lithography: A Comparison of Reactive Magnetron Sputtering and HiPIMS<br>*Aristotle University of Thessaloniki, Greece* |
| **11h40** | *S4-02* - **Karmen Kapustic**<br>From Growth to Strain: Temperature Dependent MoS2 Island Formation on Graphene/Ir(332)<br>*Centre for Advanced Laser Techniques, Institute of Physics, Croatia* |
| **12h00** | *S4-03-* **Andrea Besana**<br>Low temperature deposition of germanium for SWIR monolithic photodetector integration<br>*Politecnico di Milano, Italy* |
| **12h20** | **Lunch** |
| **14h20** | *S5-01* - **Gamze Yolcu**<br>MOVPE Growth and Doping Optimization of n-AlGaAs Layers for Laser Diodes<br>*Sivas Cumhuriyet University, Turkey* |
| **14h40** | *S5-02* - **Evelina Dudutienė**<br>Effect of growth and annealing on emission from parabolic GaAsBi/AlGaAs quantum wells<br>*Center for Physical Sciences and Technology, Lithuania* |
| **15h00** | *S5-03* - **Aistė Štaupienė**<br>Quantitative IQE Analysis of GaAsBi/GaAs MQWs<br>*SRI Center for Physical Sciences and Technology, Lithuania* |
| **15h20** | *S4.04* - ***Eva Monroy - Invited Speaker***<br>MBE-grown AlGaN Nanostructures for UV Emitters<br>*CEA-Grenoble, France* |
| **16h00** | **Coffee Break** |
| **16h40** | *S6-01* - **Giulio Senesi**<br>Structural and Transport Properties of Thin InAs Layers Grown on InxAl1−xAs Metamorphic Buffers<br>*Istituto Nanoscienze-CNR and Scuola Normale Superiore, Italy* |
| **17h00** | *S6-02* - **Izel Perkitel**<br>*AlN Schottky Barrier Diodes: Epitaxial Growth and Characterization*<br>*Sivas Cumhuriyet University, Turkey* |
| **17h20** | *S6-03* - **Stefan Heun**<br>Superconducting Quantum Interference Devices based on InSb Nanoflag Josephson Junctions<br>*Instituto Nanoscienze-CNR and Scuola Normale Superiore* |
| **17h40** | *S6-04* - **Mahmoud M. Youssif**<br>Efficient adsorption of Cd2+ and Pb2+ ions from wastewater using a novel Fe3O4@SiO2/PANI-SDBS nanocomposite<br>*AGH University of Krakow, Poland* |

## May 21, 2025

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| **8h30** | **Registration** |
| **9h00** | *S7-01* - **Beatriz Galiana Blanco**<br>STEM characterization of III-V nanowires using 4D STEM and Differential Phase Contrast<br>*Universidad Carlos III de Madrid, Spain* |
| **9h20** | *S7-02* - **Emanuele Pompei**<br>STM investigation of novel structures of Gallenene intercalated in epitaxial Graphene<br>*NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, Italy* |
| **9h40** | *S7-03* - **Martynas Skapas**<br>In-situ TEM investigation of Bi quantum dots formation<br>*Center for Physical Science and Technology, Lithuania* |
| **10h00** | *S7.04* - ***Miroslav Kolíbal - Invited Speaker***<br>Real-Time Study of Surface-Guided Nanowire Growth by In Situ Scanning Electron Microscopy<br>*Brno University of Technology, Czech Republic* |
| **10h40** | **Coffee Break** |
| **11h20** | *S8-01* - **Jonas Johansson**<br>Heteroepitaxial Growth Modes Revisited<br>*Lund University, Sweden* |
| **11h40** | *S8-02* - **Man Suk Song**<br>Topotactic Growth of Eu-based Zintl-phase Nanowires and Thin Films by Molecular Beam Epitaxy<br>*Weizmann Institute of Science, Israel* |
| **12h00** | *S8-03* - ***Raffaella Calarco - Invited Speaker***<br>Van der Waals Epitaxy and Characterization of Quasi Two-Dimensional Ge-Sb-Te Materials<br>*CNR - Institute for Microelectronics and Microsystems, Italy* |
| **12h40** | **Lunch** |
| **14h20** | *S9-01* - **Zoran Jovanovic**<br>PLD-based integration of strontium titanate thin films with silicon substrate for robust solar water splitting<br>*Laboratory of Physics, Vinča Institute of Nuclear Sciences, Serbia* |
| **14h40** | *S9-02* - **Thomas Dursap**<br>SiGe:B Source/Drain epitaxy for advanced device applications<br>*Imec, Leuven, Belgium* |
| **15h00** | *S9-03* - **Bogdana Borca**<br>Manipulating Electronic and Magnetic Properties of a 2D Antiferromagnetic Material through Interface Effects<br>*National Institute of Materials Physics, Magurele, Romania* |
| **15h20** | *S9-04* - ***Charles Cornet - Invited Speaker***<br>Cost-effective solar water splitting with III-V/Si epitaxial photoelectrodes<br>*Institut FOTON, France* |
| **16h00** | **Coffee Break** |
| **16h40** | *S10-01* - **Cosmin Romanitan – STSM**<br>High-photocatalytic activity of PA-MBE grown GaN nanowires for degradation of methylene blue<br>*National Institute for Research and Development in Microtechnologies, Romania* |
| **17h00** | *S10-02* - **Francesco Salutari – STSM**<br>Investigating the Oxidation/Reduction Mechanism of Zinc Phosphide by In-Situ Transmission Electron Microscopy<br>*Catalan Institute of Nanoscience and Nanotechnology, Spain* |
| **17h20** | **Poster Session** |

## May 22, 2025

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| **8h30** | **Registration** |
| **9h00** | *S11-01* - **Giada Bucci**<br>Tunable GaAsxP1-x Quantum-Dot Emission in Wurtzite GaP Nanowires<br>*NEST, Scuola Normale Superiore and Istituto Nanoscienze, Italy* |
| **9h20** | *S11-02* - **Aurelian Catalin Galca**<br>Colossal magnetoresistance at room temperature of manganese-based perovskite epilayers grown on 001 SrTiO3 substrates<br>*National Institute of Materials Physics, Magurele, Romania* |
| **9h40** | *S11-03* - **Lenka Zajickova**<br>Optical Properties of Nitrogen-Doped Carbon Quantum Dots<br>*CEITEC, Brno University of Technology, Czechia* |
| **10h00** | *S11-04* - ***Anna Musial - Invited Speaker***<br>Optical properties and electronic structure of zinc-blende $In_xAs_{1-x}P$/InP quantum dots in nanowires emitting at telecom wavelengths<br>*Department of Experimental Physics, Faculty of Fundamental Problems of Technology, Poland* |
| **10h40** | **Coffee Break** |
| **11h20** | *S12-01* - **Arturs Medvids**<br>Mechanism of Ge Quantum Cones Formation by Laser Radiation on a Surface of SiGe/Si Solid Solution Grown by Molecular Beam Epitaxy<br>*Laboratory of Semiconductor Physics, Riga Technical University, Latvia* |
| **11h40** | *S12-02* - **Cosme Gonzalez Ayani**<br>Comparative Study of $VS_2$ Epitaxy on Strained and Relaxed Graphene<br>*Center for Advanced Laser Techniques, Institute of Physics, Croatia* |
| **12h00** | *S12-03* - **Gaurav Shukla**<br>Tunable Superconducting Transport in 2D-InSb/Nb-based Hybrid Josephson Junctions with Dual-Gate Electrostatic Control<br>*NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, Italy* |
| **12h20** | *S12-04* - **Nuno E. Silva**<br>Energy storage properties in ferroelectric epitaxial La:HfO2 based thin film capacitors<br>*Physics Center of Minho and Porto Universities, Portugal* |
| **12h40** | **Lunch** |
| **14h20** | *S13-01* - **Marta Chabowska**<br>Mechanisms of Meander Formation: The Role of Surface Energy Potential<br>*Institute of Physics, Polish Academy of Sciences, Poland,* |
| **14h40** | *S13-02* - **Jayakrishnan Ampattu Ravikumar**<br>Engineering relaxor ferroelectric epitaxial thin films for low voltage energy storage applications<br>*Physics Center of Minho and Porto Universities, Portugal* |
| **15h00** | *S13-03* - **Aleksandra Nadolska**<br>Resistive switching in 2D MoO3 studied by atomic force microscopy<br>*Faculty of Physics and Applied Informatics, University of Lodz, Poland* |
| **15h20** | *S13-04* - ***Iva Šrut Rakić - Invited Speaker***<br>Engineering Strain in 2D Materials: Surface Interactions and Substrate Modification<br>*Centre for Advanced Laser Techniques, Institute of Physics, Croatia* |
| **16h00** | **Coffee Break** |
| **16h40** | *S14-01* - ***Carlos Felipe Blanco Rocha - Invited Speaker***<br>Safe and sustainable-by-design approaches to epitaxial PV cells<br>*Institute of Environmental Sciences & Netherlands Organisation for Applied Scientific Research, The Netherlands* |
| **17h00** | *S14-02* - ***Bruno Gayral - Invited Speaker***<br>Considerations on the rebound effects and the technological promise<br>*CEA-Grenoble, France* |
| **17h20** | **Round Table** |

## May 23, 2025

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| **8h30** | **Registration** |
| **9h00** | |
| **9h20** | *S15-01* - **Aivaras Špokas**<br>Strategies for Improvement of GaAsBi Quantum Well-Based Laser Performance for Emission above 1000 nm<br>*Center for Physical Sciences and Technology, Vilnius, Lithuania* |
| **9h40** | *S15-02* - **Dudu Hatice Ünal**<br>Optimized MSM Photodetector Design: The Influence of Barrier and Digital Graded Superlattice Layers<br>*Sivas Cumhuriyet University, Turkey* |
| **10h00** | *S15-03* - **Adnan Kareem**<br>Fabrication and Characterization of Iron Titanate Thin Films as a Potential Tunnel Barrier for Magnetic Tunnel Junction (MTJ’s)<br>*Institute of mathematics physics and mechanics, Slovenia* |
| **10h20** | *S15-04* - **Alejandro Plaza**<br>Epitaxial Growth of LSMO Thin Films by Solid State Pulsed Laser Deposition for MEMS Applications<br>*CNR-SPIN, Genova, Italy* |
| **10h40** | **Coffee Break** |
| **11h20** | *S16-01* - **Ifra Saeed**<br>Electrodeposited Zirconium Titanate Thin Films: Structural, Magnetic, and Dielectric Properties for Spintronic Applications<br>*Department of Physics and Astronomy, University of Milano Bicocca, Italy* |
| **11h40** | *S16-02* - **Afonso De Cerdeira Oliveira**<br>Ge-on-Si dual-band detectors for solvents recognition<br>*LNESS Dipartimento di Fisica, Politecnico di Milano, Italy* |
| **12h00** | *S16-03* - **Lala Gahramanli**<br>Advanced Functional CdxZn1-xS Nanocomposites: Comparative Study of Sonochemical and SILAR Synthesis for Application-Oriented Materials<br>*Nano Research Laboratory, Azerbaijan* |
| **12h20** | **End - few words** |

## Poster session – May 21, 2025

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| *PS.01* | FeGa/MoSe2/hBN and AlOx/FeGa/MoSe2/hBN heterostructres for combination of magnetostriction effects with 2D materials<br>**Ali Ercetin**<br>*Bandırma Onyedi Eylul University, Turkey* |
| *PS.02* | FDTD simulations of InxAs1-xP quantum dots in zinc-blende InP nanowires for efficient telecom band emission<br>**T. Gzyl**<br>*Faculty of Fundamental Problems of Technology, Wrocław, Poland* |
| *PS.03* | Ranges and limits of p-doping in Y:HfO2 – an electronic structure study by HAXPES<br>**Oliver Rehm**<br>*Universität Konstanz, Germany* |
| *PS.04* | Second-order Phase Transition and Magnetic Anisotropy-Driven Magnetocaloric and Giant Magnetoresistance Effects in La-Ba-Mn-Ti-O Epitaxial Thin Films<br>**Marwène Oumezzine**<br>*Laboratoire de Physico-Chimie des Matériaux, Tunisia* |
| *PS.05* | Growth optimization of Sb2Se3 thin films on ZnSe/ITO substrates<br>**Tamara Potlog**<br>*Laboratory of Organic/Inorganic Materials for Optoelectronics, Moldova State University* |
| *PS.06* | Low-temperature growth of Al monolayer on 7×7 reconstructed Si (111) surface by molecular beam epitaxy<br>**Nhu Tran**<br>*Institute of Physics of Materials and CEITEC IPM, Czech Republic* |
| *PS.07* | Fabrication of blue phosphorene<br>**J. David**<br>*Institute of Physical Engineering and Nanotechnology, Czech Republic* |
| *PS.08* | Single-phase κ-Ga2O3 films deposited by Metal-Organic Vapor Phase Epitaxy on GaAs and ternary BxGa(1-x)As templates<br>**Tarak Hidouri**<br>*Department of Mathematical, Physical and Computer Sciences, University of Parma, Italy* |
| *PS.09* | Energy storage and harvesting performance of Aurivillius oxide thin films grown by pulsed laser deposition<br>**Boutheina Abdellaoui**<br>*Laboratoire de Physique Appliquée, Université de Sfax, Tunisia* |
| *PS.10* | Impact of Bismuth Dopant Layers on the Optical Behavior of GaAs/AlAs Quantum Wells<br>**Justas Žuvelis**<br>*State research institute Center for Physical Sciences and Technology, Lithuania* |
| *PS.11* | Growth and transfer approaches to back-gated oxide heterostructure devices<br>**K. Nayak**<br>*Peter Grunberg Institute, Juelich, Germany* |
| *PS.12* | Mechanisms of Temperature-Dependent CO Adsorption on BaTiO3(001): Surface Stability and Gas Sequestration Potential<br>**D.G. Popescu**<br>*National Institute of Materials Physics, Ilfov, Romania* |

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| *PS.13* | Direct growth and application of 2D single crystals of MXenes<br>**Pranjali Jadhao1**<br>*CEITEC BUT, Brno University of Technology, Czech Republic* |
| *PS.14* | AlGaN buffer layers grown on sapphire substrates<br>**J. Batysta**<br>*FZU - Institute of Physics, Czech Republic* |
| *PS.15* | Thick InGaN layers for water photocatalysis grown on sapphire substrate by MOVPE<br>**Markéta Slavická Zíková**<br>*Institute of Physics, Czech Academy of Sciences, Czech Republic* |
| *PS.16* | Fully digital 3D imager for hard X-rays: MBE growth and fabrication challenges<br>**Matias Antonelli**<br>*INFN, Sezione di Trieste, Italy* |
| *PS.17* | Epitaxial Growth of Iron and Cobalt on Oxide Substrates<br>**Adina Diana Dobrin**<br>*National Institute of Materials Physics, Romania* |
| *PS.18* | SiGe PIC sensor<br>**Vittoria Urso**<br>*Dipartimento di Fisica”E. Fermi”, Università di Pisa, Italy* |
| *PS.19* | Unexpected trench self-patterning in InGaAs/InP: a route to pseudo-substrates for 2 µm applications<br>**C. Barbier**<br>*Tyndall National Institute, Cork, Ireland* |
| *PS.20* | MoS2/PtX2 van der Waals heterostructures<br>**Dimitre Dimitrov**<br>*Institute of Solid State Physics-Bulgarian Academy of Sciences, Bulgaria* |
| *PS.21* | Pt- and Pd- based noble-metal dichalcogenides<br>**Vera Marinova**<br>*Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, Bulgaria* |
| *PS.22* | Transmission Electron Microscopy Analysis of Ga2O3 Thin Films Homoepitaxially Grown on (010), (-201) and (001) Substrates<br>**Vincent Sallet**<br>*Groupe d’Etude de la Matière Condensée CNRS, Université de Versailles, France* |
| *PS.23* | MOCVD growth of ZnxCd(1-x)S epilayers on non-polar m-plane and a-plane wurtzite CdS substrates<br>**Gaelle Amiri**<br>*Groupe d’Etude de la Matière Condensée CNRS, Université de Versailles, France* |
| *PS.24* | Ge and GeSn NWs for group IV Photonic applications<br>**Ludovica Lunghi**<br>*Laboratory of Semiconductor Materials, Ecole Polytechnique Fédérale de Lausanne, Switzerland* |

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# Taking the Crystal Growth of $Cu_2O$ to a New Level

M.Zervos[1*], K.Koutsokostas [2], N.Florini [2], P.Komninou [2], N.Lathiotakis [3], I.Paschos [4], P.Savvidis [4]

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*[2]Department of Condensed Matter and Materials Physics, School of Physics, Aristotle University of Thessaloniki, GR-54124, Thessaloniki, Greece.*
*[3] Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Vass. Constantinou 48, GR-11635 Athens, Greece.*
*[4] International Center for Polaritonics, Department of Physics, Westlake University, Zhejiang, Hangzhou, Xihu, 310024, China*
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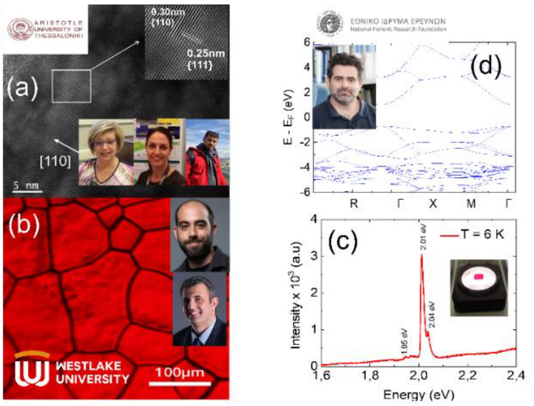
Keywords: Cuprous Oxide, Crystal Growth

$Cu_2O$ is a p-type metal oxide semiconductor that has a cubic crystal structure and a direct energy band gap of 2.1 eV. It is an archetype for the study of excitons especially after the observation of giant Rydberg excitons with principal quantum numbers up to n = 25 by Kazimierczuk *et al.*[1] which instigated further interest into the possibility of adding long-range interactions to the physics of exciton-polaritons that were recently detected in a $SiO_2/Ta_2O_5/Cu_2O/Ta_2O_5/SiO_2$ Fabry-Pérot cavity by Orfanakis *et al.*[2] However, so far, giant Rydberg excitons and polaritons have only been observed in naturally occurring crystals of $Cu_2O$, so it is necessary to grow high quality, single crystals, of $Cu_2O$, which is interesting not just from a fundamental but also technological point of view i.e. for the fabrication of solar cells and photocatalysis. In this talk I will describe the difficulties involved with the growth of single crystal ingots and wafers of $Cu_2O$ and identify the most important bottlenecks that need to be overcome in order to improve the quality of this novel p-type metal oxide semiconductor. To this end I will describe recent advances [3] in attaining high crystal quality and purity thin wafers of $Cu_2O$ that are suitable for the epitaxial growth of other oxides and the fabrication of cavities and devices. In addition to the issues related to growth I will be describing the structural and optical properties of the $Cu_2O$ crystals [3] as shown in Figure 1 as well as future work directions that will take it to an entirely new level.



**References**

[1]Kazimierczuk, T.; Fröhlich, D.; Scheel, S.; Stolz, H.; Bayer, M. Giant Rydberg excitons in the Copper Oxide $Cu_2O$, *Nature* **2014**, *514*, 343–347.

[2]K. Orfanakis, S.K. Rajendran, V. Walther, T. Volz, T. Pohl, H. Ohadi, Rydberg Exciton–Polaritons in a $Cu_2O$ Microcavity, *Nat. Mater.*, 2022, **21**, 767–772.

[3]M.Zervos, N.Lathiotakis, K.Koutsokostas, N.Florini, P.Komninou, P.Savvidis, I.Paschos, High crystal quality and purity $Cu_2O$ by consecutive in situ annealing and thermal oxidation of Cu under $H_2$ and $O_2$ at elevated temperatures *RSC, Cryst.Eng.Comm,* 2025.

# Extreme doping of GaN with Si and Ge by plasma-assisted molecular beam epitaxy

M. Sawicka*, H. Turski, G. Muzioł, M. Siekacz, A. Feduniewicz- Żmuda, O. Gołyga,
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N-type doping of gallium nitride (GaN) is relatively straightforward in plasma-assisted molecular beam epitaxy (PAMBE). Incorporation of Si or Ge dopant atoms scales linearly with the flux for a wide range of concentrations and high crystalline quality is preserved. However, for some particular applications, higher doping levels $>1\times10^{20}$ cm$^{-3}$ would be beneficial, e.g. for low-voltage tunnel junctions[2] or efficient microLED transfer enabled by selective electrochemical etching [3]. Such high doping levels pose several questions regarding crystal quality, electrical properties and doping profile abruptness.

This work presents peculiarities of Si and Ge doping in PAMBE with special focus on the extreme doping regime > $1\times10^{20}$cm$^{-3}$. First, we observed that high Si-doping from $1\times10^{19}$ to $1\times10^{20}$cm$^{-3}$ promotes hillock formation in GaN:Si$^{++}$ grown under metal-rich conditions on sapphire templates. Hillock arms incorporate more point defects and/or neutral complexes of Si with vacancies. This is evidenced with the aid of electrochemical etching (ECE) that is sensitive to the electrical properties of a layer in a nanoscale and reveals beautiful "nanostars" – see Figure 1[1], that can be detrimental for achieving electropolishing. For GaN:Si homoepitaxy we also observe non-uniform etching patterns related to step-bunching[4].

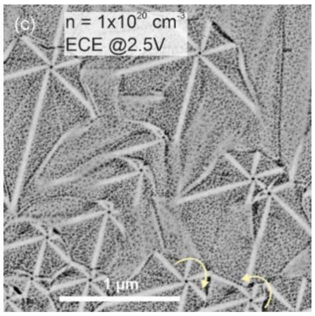

*Figure 1. GaN:Si layer n=1×10$^{20}$cm$^{-3}$ after ECE that revealed nano-inhomogeneities in electrical properties related to hillocks[1].*

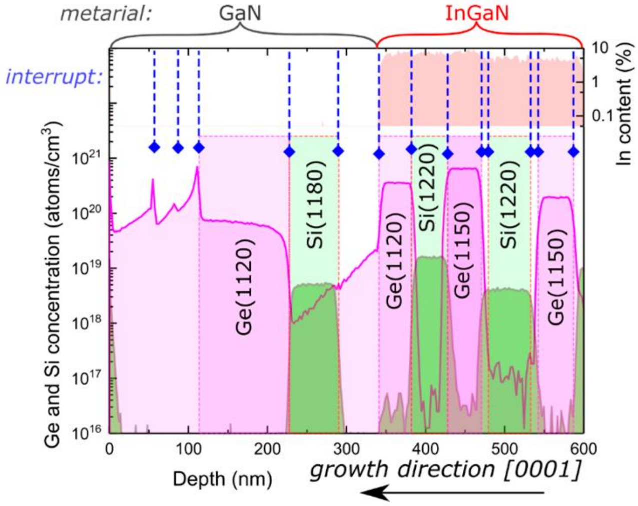

*Figure 2. SIMS profile of an GaN/InGaN layer stack showing abrupt doping interfaces for GaN:Si, InGaN:Si and InGaN:Ge, in contrast to GaN:Ge[5].*

In the second part, we will present the capability of MBE to dope GaN with Ge to extremely high levels, up to $7.9\times10^{20}$cm$^{-3}$ and show the device applications of such doping. Interestingly, when GaN:Ge is grown with gallium as a surfactant, there is a tendency for Ge to stay in the gallium surface adlayer. Then, a "memory effect" for Ge doping is observed in the GaN layer grown on top even though the Ge flux is no longer supplied from the effusion cell. Abrupt doping profiles are achieved only for InGaN:Ge[5], see Figure 2. Last but not least, GaN:Ge and GaN:Si electrical characterization will also be discussed and compared to complementary growth techniques[6].

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# Epitaxial Growth of Iron and Cobalt on Oxide Substrates

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Keywords: Molecular Beam Epitaxy, Low Energy Electron Diffraction, X-Ray Photoelectron Spectroscopy

Molecular beam epitaxy (MBE) is a highly precise technique for the deposition of thin films, enabling the controlled layer-by-layer growth of materials with atomic-level precision under ultra-high vacuum conditions. MBE facilitates epitaxial alignment between the deposited film and the substrate, making it a pivotal method for fabricating advanced heterostructures such as GaAs/AlGaAs and GaN/AlBaN, which are essential for optoelectronic devices and high-performance transistors. The precise control offered by MBE enables the tailoring of layer compositions and thicknesses at the atomic scale, allowing for the optimization of electronic properties and quantum effects in advanced semiconductor applications. Despite its remarkable precision, molecular beam epitaxy faces challenges such as maintaining ultra-high vacuum conditions and controlling the purity of source materials, both of which are critical for achieving defect-free heterostructures. Additionally, the complexity of managing interfacial strain and lattice mismatches between layers limits the range of compatible substrate-material combinations, posing further obstacles to optimizing the performance of electronic devices. Here, we report a new, easier method to grow transition metals on oxides from oxyhydroxides precursors. Focusing on FeOOH and CoOOH deposited by chemical methods on SrTiO3 (STO) substrates, we achieve epitaxial Fe and Co layers by series of flash annealing. The resulting films exhibit remarkable surface crystallinity, as evidenced by the high-quality LEED patterns shown below.
Our newly developed technique could be easily extended to other materials and substrates.

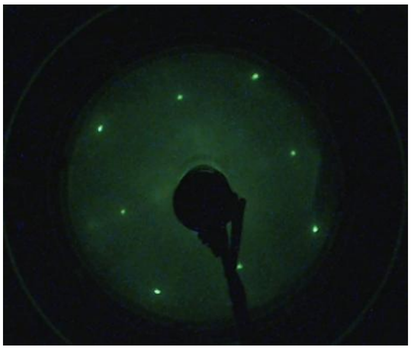

*Figure 1 Fe on STO(001)*

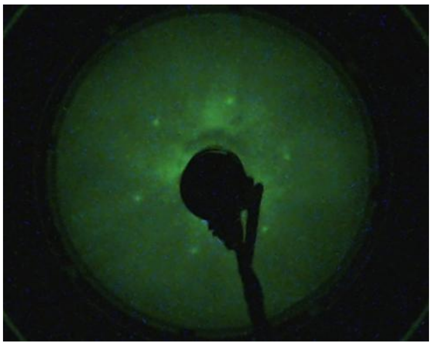

*Figure 2 Fe on STO(111)*

Funded by the European Union

# Novel growth method for TiN on GaAs(001) and $TiO_2$

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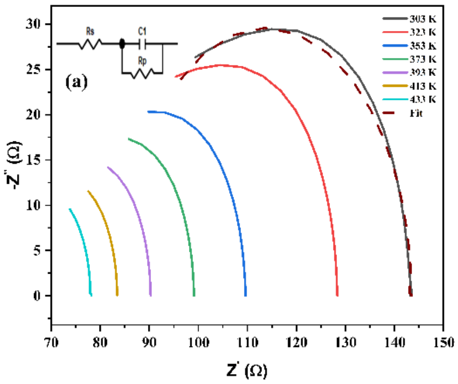
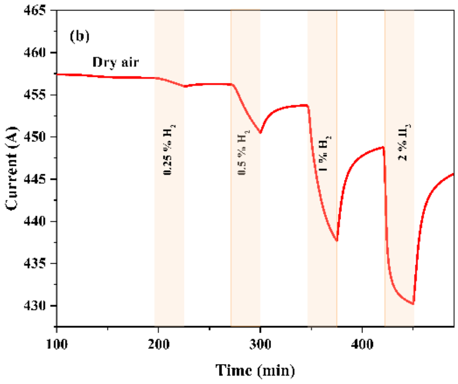
Keywords: IBPVD method, TiN thin film, $TiO_2$ nanotube, $H_2$ sensor





Titanium nitrides, oxides, and oxynitrides (TiN, $TiO_2$, and $TiN_xO_y$) are widely explored for their potential applications in energy storage, solar cells, sensors, protective coatings, and electrocatalysis. In this study, we introduce a novel growth method for TiN thin films on GaAs(001) and $TiO_2$ nanotube substrates using an innovative ion beam asisted physical vapor deposition (IBPVD) technique. This approach employs a cold cathode ion gun, typically used for Ar sputter cleaning, operated with $N_2$ gas, along with a modified titanium sublimation pump as a Ti source. $TiO_2$ nanotubes were firstly synthesized via electrochemical anodization in an ethylene glycol-based electrolyte at 40 V for 2 hours, serving as a template for TiN deposition. The thickness of TiN films was systematically varied to optimize material properties. Comprehensive structural and electrical characterization was conducted using X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), energy dispersive X-ray spectroscopy (EDS), and X-ray photoelectron spectroscopy (XPS). FE-SEM and EDX analyses confirm that TiN is uniformly and homogeneously deposited on both the GaAs surface and $TiO_2$ nanotubes. Nyquist plot (Figure a) shows a series resistance ($R_s$) and a parallel resistance-capacitance network, where the semicircle diameter decreases with increasing temperature, indicating enhanced charge transfer. The gas-sensing properties of the TiN samples were evaluated under different hydrogen ($H_2$) concentrations. A noticeable drop in current is observed as the hydrogen concentration increases, indicating strong adsorption and reaction at the sensor surface. The results demonstrate that the TiN films grown using this novel IBPVD method exhibit high crystallinity, uniform morphology, and strong interfacial adhesion, making them promising for advanced sensor and electronic applications.

# Rotational domains in epitaxial $Ga_2O_3$: identification of their origin and new strategies to prevent them.

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Keywords: $Ga_2O_3$ polymorph, Rotational domains, $Al_2O_3$ substrates, Metalorganic Vapour-Phase Epitaxy, X-Ray Diffraction, Scanning Electron Microscopy.

Gallium Oxide (especially the monoclinic $\beta$-$Ga_2O_3$ polymorph) is an ultrawide bandgap semiconductor with interesting application in the field of power electronics and UVC light detection. Despite the great deal of research, there are several issues to be solved before fully exploiting the potential of this material. One of these is the occurrence of rotational domains in films epitaxially grown on commercial substrates with hexagonal crystal lattice, like c-oriented $\alpha$-$Al_2O_3$ or 4H-SiC sapphire. These rotation domains indeed adversely affect the in-plane conductivity of the material. They are caused by the equally-probable nucleation of monoclinic $\beta$-$Ga_2O_3$ islands rotated by 120° around the (0001) direction of $\alpha$-$Al_2O_3$. The purpose of this research is to test alternative substrate orientations, i.e. the A-, M- and K-planes of sapphire and find optimized growth conditions in order to have a pure $\beta$ phase with lower, or even no, occurrence of rotational domains. A series of $\beta$-$Ga_2O_3$ films were deposited at different temperatures by MOVPE on 2” A-plane (11-20) and C-plane (0001) $\alpha$-$Al_2O_3$ substrates. Extensive characterisations by X-ray diffraction (XRD) revealed that the film/substrate interface is made of a mixture of $\alpha$- and $\beta$-phase grains, while the upper part of the film is pure phase $\beta$. A substrate temperature of 840°C seems to increase the possibility of obtaining a pure phase interface layer. Further research will focus on the optimization of crystal quality and on the investigation of the electrical properties of these samples. The deposition on other $Al_2O_3$ planes will also be explored to check their suitability for domain-free epitaxial growth.

# Optimization of Growth Parameters in the LPCVD of UWBG Rutile Germanium Dioxide

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Keywords: Chemical vapor deposition, CVD, ultra-wide energy bandgap, UWBG, rutile germanium dioxide, r-$GeO_2$

Ultra-wide bandgap (UWBG) semiconductors, characterized by an energy bandgap exceeding 3.5 eV, have recently garnered significant attention for their potential applications in next-generation radio frequency (RF) devices, power electronics, and deep-ultraviolet (deep-UV) optoelectronics. Recent theoretical studies have indicated that rutile germanium dioxide ($GeO_2$) possesses an energy bandgap of 4.68 eV and exhibits ambipolar doping capability, along with satisfactory electron and hole mobility.

There has been recent efforts for both melt and and thin film growth development of r-$GeO_2$ . Using flux method very small size single crystals have been grown with very low growth rates. In the thin film growth side, many growth systems have been used such as molecular beam epitaxy (MBE), metal organic chemical vapor deposition (MOCVD), pulsed laser deposition (PLD), Mist-CVD. Unfortunately, all reported attempts to achieve single-crystal rutile $GeO_2$ have relied exclusively on rutile $TiO_2$ substrates, which are not only costly but also commercially available in limited sizes, with a maximum diameter of approximately 2 inches. Additionally, the growth rate for achieving reasonably high-quality layers has been found to be restricted to ~50 nm/hr, which is relatively low and poses a significant limitation for optoelectronic and power electronic device applications.

In this work, we explore the low-pressure chemical vapor deposition (LPCVD) system for the growth of (101) oriented r-$GeO_2$ on a-plane sapphire which is cheap and available in large size. We use solid sources of Ge granules and $GeO_2$ powder, gas sources of $O_2$ and Ar in the growth. Independently controlling source and substrate temperatures and transferring $O_2$ to the substrate in a close coupled design enables the adjustment of growth parameters efficiently. We have explored the effects of substrate and Ge source temperature, reaction pressure, $O_2$ and Ar flow rates on the structural properties of the samples. By tunning these parameters, we could tune the growth rate, suppress the growth of h-$GeO_2$. We could achieve growth rates up to 2.2 μm/hr, far exceeding the typical thin film growth rates in the literature. Samples with on-axis XRD rocking curve fwhm of 511 arcsecs could be achieved. STEM measurements revealed the reduction of dislocations as the film gets thicker with highly ordered crystalline r-$GeO_2$ structure. To conclude, this work explored the LPCVD growth window for the development of high quality (101) r-$GeO_2$ on a-sapphire substrates by effectively tuning growth parameters.

This study was supported by Scientific and Technological Research Council of Turkey (TUBITAK) under the Grant Number 121F371.

# Segregation-driven formation of Bi-QDs in GaAsBi layered structures

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Keywords: GaAsBi, Bi QDs, phase diagram, TEM, PL

Very intensive investigation of GaAsBi alloy, exhibiting efficient energy bandgap reduction (up to 88 meV/%Bi) and low sensitivity to temperature, revealed several potential bismide applications in NIR photonics. The technological challenges - low epitaxy temperature and close to 1 As to Ga ratio - lead to poor crystalline quality and weak luminescence [1, 2]. Moreover, Bi segregation at high temperatures generates droplets in the interfaces and on the surface. All these peculiarities held-back wider bismide applications. Althoug, the attempts to anneal demonstrated different findings: (i) the improved GaAsBi crystalline structure and (ii) formation of nanometer-size pure Bi crystals, many fundamental questions remain still unclear. Thus, the thermodynamic stability of solid solutions, in particular, quantitative estimates of the expansion of the immiscibility region, is one of the main subject of consideration [3, 4].

This work is focused on the investigation of alternative Bi QDs formation mechanism using segregation process performing annealing of GaAsBi layers and quantum structures. The obtained TEM images demonstrated that annealing in MBE reactor at 750 ºC for 0 – 150 s results in the formation of randomly oriented Bi QDs with a dominating size of about 10 – 15 nm. Optical characterization revealed the impact of annealing time and temperature for Bi segregation process and QDs formation, demonstrating the redshift, intensity reduction and broadening of emission measured from GaAsBi layer, and PL enhancement from Bi QDs.

Based on thermodynamic analysis, the phase stability of the pseudobinary semiconductor GaAsBi/GaAs alloys was modelled. Obtained T-x phase diagrams allowed to predict the existence of the wide miscibility gap. Taking into account the internal stresses and the influence of GaAs substrate, the significant change for small Bi content comparing to the bulk was determined in the phase diagram. The narrowing of the immiscibility region was demonstrated experimentally also [5]. The evaluated critical temperature Tc-2113 K and thickness dependence on Bi content in GaAsBi correlate well with the results of first-principles calculations (Tc = 2097K) [5] and experimental thickness investigation results [6,7].

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# GaP on Si integration by chemical beam epitaxy

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Keywords: Chemical beam epitaxy, Si epitaxy, III-V on Si

GaP on Si virtual substrates or templates are very interesting because they can reduce the final price of III-V devices. However, Si native oxide and hydrocarbon surface contamination must be removed before the epitaxial growth of a Si buffer layer, also avoiding any intermediate air exposure in order to obtain a clean and smooth Si surface. Gaseous precursors used in chemical beam epitaxy (CBE) of Si should be carbon-free to prevent growth inhibition due to SiC nucleation. Silanes ($Si_nH_{2n+2}$) are good candidates for Si epitaxy, but lower order silanes are highly hazardous. Nevertheless, higher order silanes are safer, as they are liquids at room temperature with sub-atmospheric vapor pressures [1], being suitable for direct injection under ultra-high vacuum without any carrier gas.

In this work, we show some results on different *ex situ* Si surface cleaning processes, as well as *in situ* moderate temperatures procedures, aiming to prepare and optimize the Si surface before the GaP buffer layer growth. Auger electron spectroscopy (AES) and reflection high-energy electron diffraction (RHEED) were used as *in situ* techniques for that purpose.

Growths were performed on nominally-oriented Si(001) substrates using trisilane ($Si_3H_8$) in a CBE system at substrate temperatures between 630 and 800 °C allowing thermal decomposition of precursor molecules on the substrate surface. After a (2×2) like surface reconstruction was observed with RHEED, specular spot intensity oscillations were monitored during Si growth, obtaining single- and double-frequency harmonics related to the growth of double ($a_0/2$) and single Si monolayers ($a_0/4$), respectively. Afterwards, without exposing the substrate to the atmosphere, a GaP buffer layer was grown at substrate temperature of 580 °C using triethylgallium (TEGa) and tertiarybutylphosphine (TBP) as precursors. A final (2×4) surface reconstruction with domains was obtained after GaP growth. AES spectra indicated no traces of oxygen or carbon on either the Si or GaP surface. Finally, the GaP/Si template was characterized by high resolution X ray diffraction (HRXRD), revealing a strained GaP layer. Antiphase domains are expected to be suppressed when using misoriented Si substrates.

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# MOVPE Optimization of InGaAs/InAlAs Superlattices: Influence of $AsH_3$ Flow and Interface Transition on Structural Properties

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Keywords: MOVPE, epitaxy, InGaAs/InAlAs superlattice, $AsH_3$ effect, transition time,

Quantum cascade lasers (QCLs) have attracted a great deal of attention since their first demonstration due to their high optical power, high efficiency, design flexibility and compactnesss [1]. While conventional semiconductor lasers rely on band-to-band recombination radiation at the junction between p- and n-type materials, QCLs emit light through electronic transitions between different energy levels within the conduction band of the semiconductor material. As a class of unipolar semiconductor lasers, QCLs play an indispensable role in many critical military and civil applications such as remote sensing, infrared countermeasure systems, thermal imaging and gas detection.

InGaAs/InAlAs-based QCL structures are widely utilized for mid-infrared wavelength emission applications. Due to the lattice compatibility of InGaAs and InAlAs with InP and the relatively mature growth and fabrication technology, InP-based QCLs are preferred. In this study, the growth and characterization of InP-based quantum cascade laser structures will be conducted. For devices with superlattice structure such as quantum cascade lasers, single layer growths do not give precise results as the relaxation mechanism dominates over the critical thickness [2]. Therefore, superlattice optimization studies should be carried out for precise growth of such devices. In this study, the effect of AsH3 flow and interface transition time on the superlattice will be investigated. In this study, $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ superlattices will be grown by Metal-Organic-Vapor-Phase Epitaxy (MOVPE) method. For the first optimization study, AsH3 flows will be grown to 47 sccm, 60 sccm and 75 sccm. For the second optimization study, the interface transition times will be scaled up to 3 s and 5 s. The studies will be analyzed structurally using a high-resolution X-ray diffractometer and optically using a photoluminescence spectrometer. Surface morphology will also be analyzed by atomic force microscopy.

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Pisa, May 2025

# Fabrication and Characterization of Germanium Nanoribbons on Aluminium (110) via Molecular Beam Epitaxy

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Keywords: Germanium Nanoribbons, Molecular Beam Epitaxy (MBE), Surface Characterization

The discovery of graphene has triggered an intense interest in low-dimensional materials [1]. Recently focus has shifted toward one dimensional 1D nanostructures for their unique electronic and quantum properties [2-4]. In this paper, we present the first successful fabrication of germanium (Ge) nanoribbons on Al(110). The surface was systematically characterized before and after germanium deposition, using X-ray photoelectron spectroscopy (XPS) to follow the chemical composition, lowenergy electron diffraction (LEED) to monitor the crystallographic structure, and scanning tunneling microscopy (STM) to visualize the surface morphology. Ge deposition was performed by molecular beam epitaxy (MBE) in a temperature range between 85°C and 300°C. We reveal that the growth of Ge on Al(110) is coverage-dependent because a transition from a (2×1) superstructure to 1D nanoribbons is observed around 1ML. Up to coverages of 0.7 ML, no structural feature change was evident. At 0.7 ML, a well-ordered (2×1) surface reconstruction becomes visible by LEED and STM. When the amount of deposited Ge exceeded 1 ML, an unexpected transformation occurred in the system. Indeed, the STM images point out the formation of parallel nanoribbons aligned along the [001] direction, with an average width of 1.5 nm and an average height of 0.22 nm, coexisting with flat unreconstructed areas. Numerical simulations provide a better understanding of the evolution of these phases. The (2×1) superstructure at 0.7 ML could be due to a succession of atomic rows predominantly and alternatively composed of Ge and Al atoms along the [-110] direction, while nanoribbon formation at higher coverages is driven by strain relief and chemical interactions. This work combines experiment and theory to understand how coverage, structure, and stability interact in 1D Ge-based systems. These findings open the way to tailor the electronic properties of nanoribbons for applications in nanoscale devices.

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# Optimization of AlGaAs Barriers in InGaAs Quantum Wells for Enhanced Near-Infrared Emission

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Keywords: MBE, Quantum Wells, NIR

Semiconductor lasers are solid state lasers that use a semiconductor gain medium, where optical amplification is achieved through stimulated emission at an interband transition. InGaAs/GaAs multi-quantum wells (MQWs) are commonly used in applications such as light emitting diodes, near-infrared lasers, photodetectors, and photovoltaic devices, owing to their high radiation efficiency and broad spectral range [1-2]. This study investigates the optimization of AlGaAs barrier compositions in InGaAs QWs to improve the optical properties.

Single InGaAs QW containing approximately 21% indium were examined with AlGaAs barriers of varying aluminum fractions (0%, 12%, 20%, and 30%). Bandedge and quantum energy levels were theoretically modeled utilizing nextnano3 software for each grown structure, revealing the dependence of energy level distributions and carrier confinement on Al content. Subsequently, molecular beam epitaxy (MBE) was employed for the growth of the quantum well structures, with precise control of growth parameters to minimize interface roughness and defects.

The structural quality and surface morphology were evaluated using atomic force microscopy (AFM), showing minimal differences in roughness among samples.

Temperature-dependent photoluminescence (PL) spectroscopy provided insights into the optical quality and efficiency of radiative recombination. At low temperatures, quantum wells with GaAs barriers exhibited superior PL, indicating fewer non-radiative recombination centers compared to Al-containing barriers. However, a significant reduction in PL intensity for GaAs-barrier samples above 200 K due to thermally activated carrier escape was observed, while AlGaAs barriers effectively maintained carrier confinement at room temperatures.

In conclusion, this optimization study clearly illustrates the trade-off between barrier height enhancement and crystal quality lowering associated with increased aluminum content. The barrier composition containing 12% aluminum was identified as optimal, combining excellent room temperature optical performance with stable carrier confinement, making it highly suitable for enhancing device performance in NIR optoelectronic applications.

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# Epitaxial Growth of β and κ $Ga_2O_3$ Polymorphs for Efficient Self-Powered p-n Photodiodes

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Keywords: $Ga_2O_3$ epilayers, Polymorph, NiO, MOVPE, photodetector, broadband, UVC

$Ga_2O_3$ has emerged as a next-generation ultra-wide bandgap semiconductor that has stimulated much research and application interest over the last decade. In particular, self-powered and efficient $Ga_2O_3$based UV photodetectors have the potential to drive significant advancements in next-generation photodetection technologies. $Ga_2O_3$ exists in five different polymorphs: α, β, γ, δ, and κ, with a bandgap energy of approximately 5 eV. UV light is commonly categorized into UV-A (320–400 nm), UV-B (280–320 nm), and UV-C (200–280 nm) regions according to radiation wavelength. In this work, we present two photodiodes based on different $Ga_2O_3$ polymorphs: κ-$Ga_2O_3$:Si/NiO for broad-UV detection (simultaneous detection of UV-A, UV-B, and UV-C) and NiO/β-$Ga_2O_3$ for selective UV-C detection. The use of the p-n heterojunction is mandatory due to the lack of p-type conductivity in $Ga_2O_3$. Heteroepitaxial growth of both β-$Ga_2O_3$ and κ-$Ga_2O_3$:Si epilayers on sapphire substrates ($Al_2O_3$) was made by metal-organic vapor phase epitaxy (MOVPE), while the NiO film was deposited on $Ga_2O_3$ via magnetron sputtering at room temperature. The structural, optical, and electrical properties of $Ga_2O_3$ polymorphs and NiO were systematically investigated. The fabricated photodiodes exhibit a compact planar-circular geometry. The κ-$Ga_2O_3$:Si/NiO photodiode demonstrates broad UV detection; the response to radiation with energy below the $Ga_2O_3$ bandgap could be attributed to the presence of deep-level traps within κ-$Ga_2O_3$:Si or to absorption within the narrow depletion region of the heavily p-doped NiO film. Conversely, the NiO/β$Ga_2O_3$ diode exhibits high selectivity to UV-C radiation with enhanced responsivity, and it is due to bandto-band excitation of photocarriers within the depletion region on the β-$Ga_2O_3$ side of the p-n junction. Additionally, both devices demonstrate fast response and recovery times (less than 0.8 s) in self-powered mode, highlighting the potential of $Ga_2O_3$-based photodiodes for high-performance UV detection applications.

# Heteroepitaxial microcrystals for infrared photonics integration

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Keywords: epitaxy on patterned substrate, Ge photodetectors, Si avalanche photodiode

The direct epitaxial growth of germanium on silicon (Ge-on-Si) has fostered the development of near infrared detectors for telecom and imaging applications. The long wavelength responsivity of these devices is limited to approximately 1550 nm corresponding to the direct energy gap of Ge. A viable route to enhance the responsivity of Gen-on-Si photodetectors in the 1550-1800 nm region, corresponding to the indirect bandgap, might be exploiting the micro-structuring of the absorbing layer to increase the optical path. In this work we report on a new type of detector, obtained from Ge micro-crystals epitaxially grown on a patterned Si substrate [1]. Figure 1 shows different crystal facet orientation that can be obtained by varying the pattern geometry. The faceted morphology and relatively high aspect ratio of the microcrystals promote light trapping-effect, enhancing the detector responsivity in the wavelength region comprised between the direct (λ≈1550 nm) and indirect (λ≈1800 nm) gap of Ge, as compared to conventional planar devices [2]. This has been exploited in photodiodes based on several microcrystals, connected in parallel by a graphene layer forming a transparent top-contact (see Fig. 2). A similar light-trapping enhancement can be observed also in homoepitaxial Si microcrystals. In this case, the larger, when compared to Ge, bandgap of Si, allows for the application of a reverse bias capable of triggering avalanche multiplication. Si-microcrystal based avalanche photodiodes (APDs) have been fabricated, demonstrating an enhancement of both, the NIR infrared responsivity and gain multiplication factor (see Fig. 3)., when compared to planar Si devices [3]

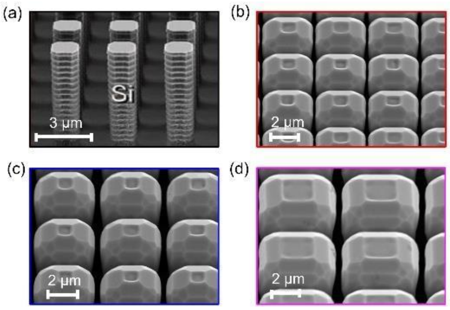

*Figure 1. Patterned Si substrate (a). Ge-on-Si microcrystals with lateral dimension W and inter-pillar gap G equal to: (b) W=2μm G=2μm , (c) W=2μm G=3μm and (d) W=3μm G=3μm.*

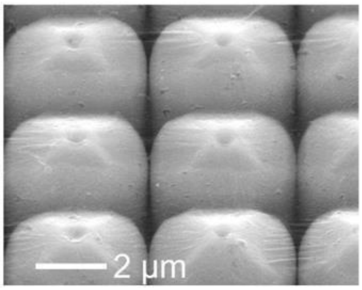

*Figure 2. Bird's eye view of a Ge microcrystal array covered by a graphene layer.*

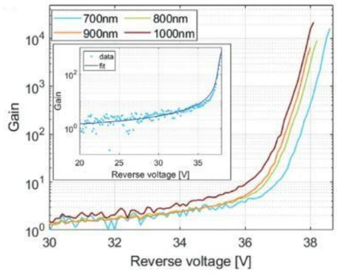

*Figure 3. Avalanche gain of microcrystals APD at different wavelengths.*

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# Challenges in the epitaxy of three-dimensional heterostructures: the case of lattice-mismatched core/shell nanowires

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Keywords: nanostructures, strain engineering, nanowire bending, growth geometry

Three-dimensional nano-heterostructures allow extreme engineering of material properties such as strain and electronic structure in semiconductors, opening up new possibilities for device applications. For example, in GaAs/$In_xAl_{1-x}As$ core/shell nanowires, depending on the In content x and the thickness of the shell, tensile strain up to unusually high values can be achieved in the core [1, 2]. This leads to significant bandgap narrowing and electron mobility enhancement in the core [1, 3], making GaAs a versatile solution for near-IR photonic applications. However, epitaxy on three-dimensional nano-objects faces challenges related to the presence of multiple growth surfaces with different orientations. This is well exemplified in core/shell nanowires grown by molecular beam epitaxy (MBE), where the shell typically exhibits inhomogeneous composition and thickness around the core, which in turn causes nanowire bending in lattice-mismatched systems.

To understand these phenomena, we have developed a model that calculates the distribution of all relevant fluxes on each side of the nanowires across the substrate, taking into account the geometry of the MBE system and all possible surface mechanisms (adatom diffusion, re-emission from the substrate, etc.) [4]. In agreement with experiments, the model shows that the typical MBE geometry inevitably leads to asymmetric shell growth around the core and bending of the nanowires, regardless of whether the substrate is rotated or not. The bending direction is determined by the geometric arrangement of the cells and the surface diffusivity of the species involved. Interestingly, In adatoms only incorporate into nanowire sides where both Al and As are present, suggesting a mechanism driven by elastic energy minimization. Similar results were obtained for $In_xGa_{1-x}As$ shells. The substrate rotation constrains the nanowire bending to the beginning of the shell growth. After a critical shell thickness, the nanowires gradually straighten, in agreement with strain-gradient calculations and measurements.

By shedding new light on the growth of core/shell nanowires and three-dimensional nanostructures in general, we hope to inspire growth strategies that provide better growth control and minimize unwanted phenomena.

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# TiN Nanotriangle Fabrication via Nanosphere Lithography: A Comparison of Reactive Magnetron Sputtering and HiPIMS

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Keywords: Titanium Nitride (TiN), Nanosphere Lithography (NSL), Magnetron Sputtering (RMS/HiPIMS)

This study investigates the fabrication of titanium nitride (TiN) nanotriangles utilizing nanosphere lithography (NSL) in conjunction with two distinct deposition techniques: reactive magnetron sputtering (RMS) and high-power impulse magnetron sputtering (HiPIMS). TiN, known for its high conductivity, hardness, and chemical inertness, is a promising material for applications in plasmonics, catalysis, and microelectronics. NSL provides a cost-effective and scalable method for creating ordered nanostructures with controlled dimensions. We explore the influence of the deposition method on the structural, morphological, and optical properties of the fabricated TiN nanotriangles.

Specifically, we compare the resulting nanotriangle arrays produced by RMS and HiPIMS, focusing on the uniformity, crystallinity, and stoichiometry of the TiN films. Atomic Force Microscopy (AFM) is employed to characterize the morphology and dimensions of the nanotriangles. Raman spectroscopy is used to determine the chemical composition and quality of TiN nanostructures. Optical properties are assessed using UV-Vis spectroscopy, examining the localized surface plasmon resonance (LSPR) characteristics of the nanotriangles.

Our findings reveal differences in the quality of the TiN nanotriangles produced by the two methods. HiPIMS, with its high ionization degree and pulsed plasma, yields films with enhanced density, smoother surfaces, and improved crystallinity compared to RMS. Conversely, RMS produces films with higher oxygen content and less defined nanostructure geometries. The impact of deposition parameters, such as sputtering power, gas flow rates, and substrate temperature, on the final nanotriangle characteristics is also discussed.

This comparative study provides valuable insights into the advantages and limitations of RMS and HiPIMS for the fabrication of TiN nanotriangles via NSL. The optimized HiPIMS process offers a route to high-quality TiN nanostructures suitable for advanced applications, contributing to the development of novel plasmonic and electronic devices.

**S4.02**

# From Growth to Strain: Temperature Dependent MoS$_2$ Island Formation on Graphene/Ir(332)

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Keywords: MoS$_2$, MBE growth, STM imaging, strain

In the field of two-dimensional (2D) materials, strain is an essential mechanism for engineering their properties, influencing their electronic and optical behavior.[1] To be able to systematically investigate the effects of strain on specific 2D materials at the nanoscale, we have developed a novel approach to inducing strain. As a case study, we present the synthesis of monolayer MoS$_2$ on a pre-patterned substrate: graphene-covered Ir(332), using molecular beam epitaxy (MBE) under ultra-high vacuum (UHV) conditions. To optimize sample quality, we studied how post-annealing temperature affects the formation of MoS$_2$ islands. A series of syntheses with varying post-annealing temperatures was performed. To assess the success of each synthesis, we conducted preliminary low-energy electron diffraction (LEED) measurements, followed by extensive scanning tunneling microscopy (STM) analysis. STM provides a variety of information, including shape and size of MoS$_2$ islands, coverage, the possible appearance of superperiodicity and lattice constant of the material. STM measurement confirmed the successful growth of MoS$_2$ island on the Gr/Ir(332) and revealed that the post-annealing temperature strongly impacts shape and size of MoS$_2$ island. At higher temperatures, we observed islands with more defined metallic edges and larger surface areas. This work highlights a successful bottom-up approach for structurally modifying and straining MoS$_2$, providing a platform for systematically studying strain-induced modifications in electronic and optical properties at the nanoscale.

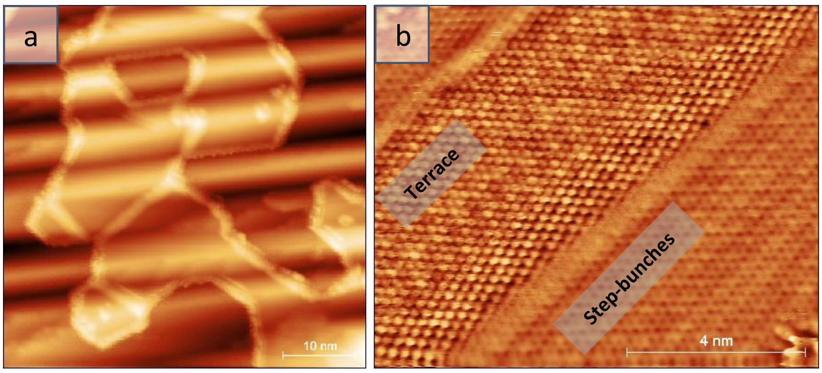

**Figure 1.** (a) STM image of a MoS$_2$ island on Gr/Ir(332) substrate, where it is visible how the material bends over the step edges. (b) STM image with atomic resolution of MoS$_2$ on different parts.

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# Low temperature deposition of germanium for SWIR monolithic photodetector integration

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Keywords: Low-T Ge epitaxy, crystal-amorphous phase transition, low thermal budget photodetector

Ge-on-Si epitaxy is a pivotal approach for emerging electronic and photonic technologies, such as infrared sensing. Nevertheless, the high growth temperature makes Ge heteroepitaxy incompatible with back-end-of-line CMOS technology. One potential solution is low-temperature (low-T) Ge deposition [1], but lower temperatures might hamper epitaxy, requiring a trade-off between CMOS compatibility and crystal quality. This work explores low-T (200-350°C) epitaxy of Ge thin films (10-250 nm), performed by Low-Energy Plasma-Enhanced Chemical Vapor Deposition.

Ge epitaxial films have been structurally characterized by HR-XRD, TEM, and Raman spectroscopy. The crystalline-amorphous phase transition was studied for samples grown at 200°C, finding out the so-called epitaxial thickness [2], after which an amorphous phase is nucleated in the growning epilayer. The complete transition occurs around 60 nm (see Raman spectra in Fig.1a and TEM image in Fig.1b). It can be concluded that the growth commences epitaxially even at 200°C and continues in a similar manner up to the epitaxial thickness. Indeed, crystalline 10 nm-thick Ge epilayers were produced. Thermal annealing can improve the crystal quality of the epilayer. This heat treatment allows the amorphous part to crystallize (solid-phase epitaxy).

Subsequently, a low-T (300°C) Ge photodiode was fabricated to demonstrate the potential process for back-end-of-line characterization. The device shows the expected rectifying behavior: the dark current density is almost two orders of magnitude larger than that of a Ge layer grown at 500°C and annealed several times at 780°C but comparable to that of a Ge-on-Si photodiode grown at 600°C without any post-growth annealing treatment, indicating that usable photodetectors can be obtained at a reduced thermal budget. It can be stated that low-T deposition at 300°C represents an optimal trade-off between a low thermal budget and a good crystal quality. This is also confirmed by the good electro-optical response of the low-T photodiode reaching a responsivity of 0.10 A/W at 1300 nm (see Fig.1c).

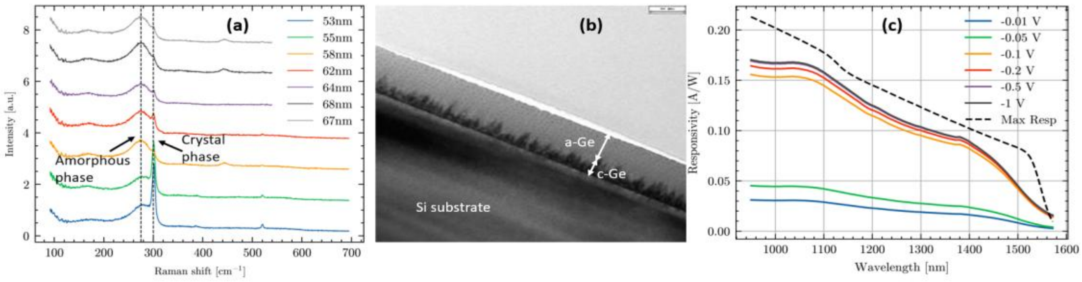

Figure 1: (a) Raman spectra of Ge crystalline-amorphous phase transition at 200°C. (b) TEM image of crystalline and amorphous interface in Ge epilayer at 200°C. (c) Measured responsivity at different bias and comparison with the maximal achievable responsivity.

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**Pisa, May 2025**

# MOVPE Growth and Doping Optimization of n-AlGaAs Layers for Laser Diodes

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Keywords: MOVPE method, $SiH_4$ doping source, epitaxial growth, carrier density

In semiconductor laser structures, epitaxial n-$Al_xGa_{1-x}As$ layers are essential components that determine both the optical and electrical performance of the device. These layers facilitate electron injection into the active region while also acting as an optical waveguide, contributing to the guidance of laser light. Since Al concentration and doping level directly affect fundamental properties such as bandgap, carrier density, and resistance losses, they must be carefully optimized. In this study, n-type $Al_xGa_{1-x}As$ layers were grown epitaxially using the MOVPE method, with $SiH_4$ gas as the doping source. To optimize doping levels, different growth parameters were tested, and HRXRD θ-2θ scans and Hall measurements were performed for each layer. The results showed that when the Al concentration exceeded 30%, the carrier density remained constant at approximately $5\times10^{17}$ $cm^{-3}$ (Figure 1). Similar trends have also been confirmed by literature studies [1,2]. To evaluate and support the accuracy of Hall measurements, ECV measurements were conducted. The analysis revealed a strong correlation between ECV and Hall measurements when the Al concentration was below 30%. However, when the Al concentration exceeded 30%, significant discrepancies were observed between the two methods. The possible reasons for these deviations were examined, and their effects on doping mechanisms and material properties were discussed. In this study, alternative methods to enhance silane doping were investigated, and strategies to be followed in case of doping failure were addressed. The results obtained were compared and evaluated with existing literature studies.

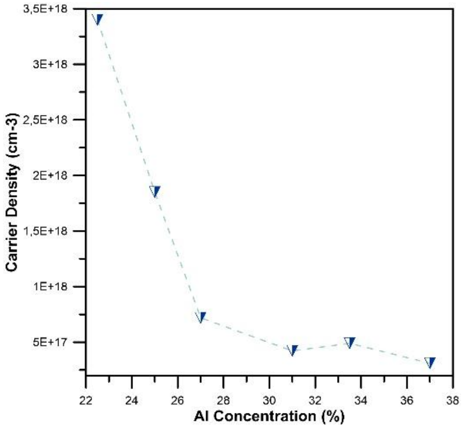

Figure 1. Variation of Carrier Density in n-$Al_xGa_{1-x}As$ Layer with Al Concentration

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Pisa, May 2025

# Effect of growth and annealing on emission from parabolic GaAsBi/AlGaAs quantum wells

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Keywords: GaAsBi, parabolic quantum wells, annealing, photoluminescence, Bi quantum dots

Lasers operating in the near-infrared (NIR) range are widely used in fields such as optical communications, remote sensing, and medicine, driving a significant demand for novel light-emitting materials tailored for NIR applications. One of the potential materials is GaAsBi. Substituting As by Bi in GaAs enables a substantial bandgap reduction while also enhancing spin-orbit splitting. Additionally, the bandgap of GaAsBi exhibits higher thermal stability compared to other materials with spectral response in the NIR range [1]. However, the growth of high-quality bismide quantum structures remains challenging due to the large Bi radius and the low growth temperatures required for Bi incorporation into the GaAs lattice.

The quality of epitaxially grown layers is typically improved through post-growth annealing at temperatures higher than the growth temperature. However, uncertainties remain regarding the effects of the annealing of GaAsBi quantum well (QW) structures. Some studies report an increase in GaAsBi emission intensity after annealing [2], while others indicate a degradation in optical quality [3]. Furthermore, in some cases, Bi nanocrystals have been observed to form within GaAsBi layer during annealing [4]. These findings suggest that the impact of annealing on GaAsBi is highly sensitive to growth conditions, making further investigation crucial for the development of GaAsBi-based NIR emitters.

This work investigates the post-growth annealing of GaAsBi QW with parabolically graded AlGaAs barriers (PGB) aiming to gain deeper insight into how these factors influence the annealing effects. PGB design was chosen to enhance photoluminescence (PL) intensity. The impact of growth conditions of parabolic AlGaAs barriers on the optical properties of annealed GaAsBi/AlGaAs QWs was investigated in detail. Notably, the substrate temperature during the growth of upper layers (above the GaAsBi) was found to significantly affect PL spectra before and after post-growth annealing. These findings highlight the importance of accounting for unintentional annealing of GaAsBi layers during the growth of full bismide-based laser structures, particularly when aiming to achieve lasers with specific performance characteristics.

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# Quantitative IQE Analysis of GaAsBi/GaAs MQWs

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Keywords: Internal quantum efficiency, GaAsBi, photoluminescence, quantum well structures

This work presents an in-depth analysis of the internal quantum efficiency (IQE) of GaAsBi quantum well (QW) structures, which are emerging as promising active media for optoelectronic devices operating in the near-infrared (NIR) region. GaAsBi/GaAs QW structures are extensively researched due to strong bandgap redshift with increasing Bi content, enhanced spin-orbit splitting and reduced temperature sensitivity [1, 2]. However, GaAsBi is a highly defective material due to its required low growth temperatures, which results in significant reduction in luminescence intensity. Therefore, optimizing the growth conditions to enhance the quality of GaAsBi structures is crucial for developing efficient NIR sources, necessitating precise efficiency measurements.

In this study, we introduce a reliable method to not only calculate the IQE (see fig. 1) but also evaluate the relative carrier recombination ratios of GaAsBi quantum structures [3]. Our results reveal that variations in growth temperature and Bi content critically affect the photoluminescence (PL) emission and, consequently, the IQE of the structures. These findings contribute to the optimization of GaAsBi growth processes, paving the way for enhanced optoelectronic device performance in the NIR region.

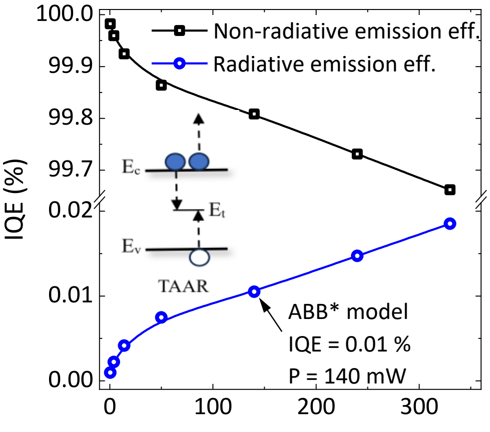

**Fig. 1.** Calculated emission efficiencies of GaAsBi/GaAs quantum well structure by ABB* model.

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S5.04

# MBE-grown AlGaN Nanostructures for UV Emitters

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Keywords: III-nitrides, nanostructures, ultraviolet, MBE

AlGaN alloys constitute the basis of today's most versatile solid-state sources of ultraviolet (UV) light, spanning the entire UVC, UVB and UVA spectral ranges through band-gap engineering. Their wide direct band gap, robust chemical stability and compatibility with both planar and three-dimensional nanostructures make AlGaN heterostructures the material platform of choice for applications such as germicidal disinfection, water purification or polymer curing. There is particular interest in two welldefined germicidal windows: the 260–270 nm range that coincides with the DNA-absorption peak, and the emerging "far-UV-C'' band at 220–230 nm, which is considered intrinsically safer for use in occupied space. Progress in metal-organic chemical vapor deposition and plasma-assisted molecularbeam epitaxy has enabled the realization of AlGaN-based LEDs, optically and electrically pumped lasers, and cathodoluminescent emitters. Yet, pushing emission below □ 300 nm while maintaining high wall-plug efficiency remains challenging because of alloy-induced point defects, parasitic polarization fields, and the tendency for transverse-magnetic light to dominate at high Al contents. Against this backdrop, quantum-confined AlGaN/AlN nanostructures—most notably quantum dots and monolayer-thin quantum wells—have emerged as powerful pathways to mitigate non-radiative recombination and tailor the optical polarization of deep-UV light.

Here we present a systematic comparison of two plasma-assisted molecular-beam-epitaxy (PA-MBE) nanostructures—Stranski–Krastanov (SK) AlGaN/AlN quantum dots (QDs) and ultra-thin GaN/AlN quantum wells (QWs). In each case, we discuss the interplay between quantum confinement, strain relaxation, and carrier localization. QDs exhibit broadband emission with internal quantum efficiency (IQE) around 50% across the full UVC window. By contrast, QW emission is highly sensitive to monolayer-scale thickness control and growth conditions. Under optimized conditions the IQE increases sharply when reducing the QW thickness, reaching 60% for single-monolayer wells emitting at 230 nm.

In summary, monolayer-scale GaN/AlN quantum wells and SK-mode AlGaN/AlN quantum dots emerge as viable, high-efficiency UV solid-state emitters. The choice between the two will ultimately be dictated by the spectral window to be addressed.

# Structural and Transport Properties of Thin InAs Layers Grown on $In_xAl_{1-x}As$ Metamorphic Buffers

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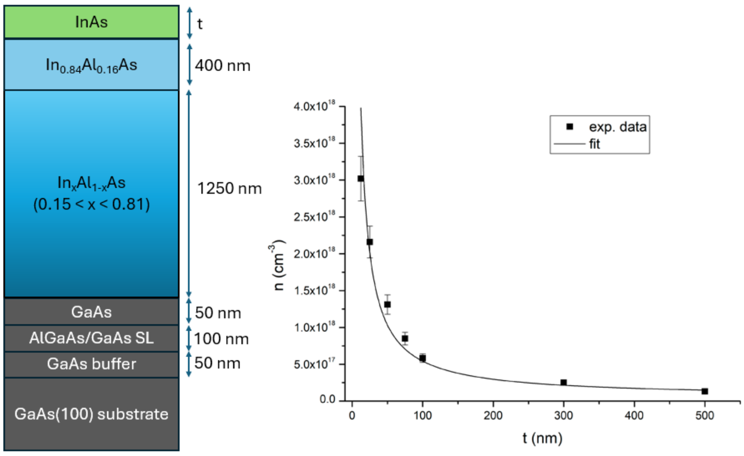
Keywords: InAs; molecular beam epitaxy; metamorphic buffers; strain; semiconductors

Indium Arsenide is a III–V semiconductor with low electron effective mass, a small band gap, strong spin–orbit coupling, and a large g-factor. These properties and its surface Fermi level pinned in the conduction band make InAs a good candidate for developing superconducting solid-state quantum devices. Here, we report the epitaxial growth of InAs layers with thicknesses ranging from 12.5 nm to 500 nm grown by Molecular Beam Epitaxy on $In_xAl_{1-x}As$ metamorphic buffers (see Figure 1(a)) [1]. The structural properties of the InAs layers were investigated by high-resolution X-ray diffraction, demonstrating the high crystal quality of the InAs layers. We performed Hall effect measurements on these samples at 300 K in the van der Pauw configuration and developed a simple two-parallel conduction model that well fits the experimental data (see Figure 1(b)). To quantify the surface charge contribution to the transport properties, two samples consisting of 50 and 100 nm thick InAs layers on a metamorphic buffer were grown with an $In_{0.84}Al_{0.16}As$ 5 nm thick cap layer on top of it, which suppresses the surface charge accumulation. The transport measurements of these two samples show that for thin layers ($t \lesssim 100$ nm), most of the charge in the InAs film is due to the surface and interface charge regions.



(a) (b)

*Figure 1*: (**a**) Sample structure of InAs on metamorphic buffer layer (InAsOI); (**b**) Carrier concentration (black square) and model fitting (solid black line).

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# AlN Schottky Barrier Diodes : Epitaxial Growth and Characterization

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Keywords: Epitaxy, AlN, Si doping, MOVPE

Recently, III-nitride semiconductors have attracted considerable interest for their applications in advanced electronic and optoelectronic devices, such as light-emitting diodes (LEDs), laser diodes (LDs), high-electron-mobility transistors (HEMTs), as well as high-power p-n and Schottky diodes. Among III-nitride semiconductors, aluminum nitride (AlN) stands out as a highly promising material for future applications, due to its outstanding properties such as a wide band gap (6.2 eV), high critical electric field strength (450 kV/cm), excellent thermal conductivity (590 W/mK), and remarkable thermal stability [1, 2].

Doping of AlN layers is crucial both for achieving the desired electrical conductivity and for controlling the carrier concentration. There are only a limited number of studies reported in the literature on the electrical conductivity in Si-doped AlN. Moreover, current research primarily focuses on using low lattice mismatch substrates, such as single-crystal AlN or SiC, to reduce dislocation defects in AlN grown by metal organic vapor phase epitaxy (MOVPE). In contrast, studies on the heteroepitaxial growth of AlN on sapphire substrates are relatively limited. However, the low cost of sapphire makes it attractive for the commercial integration of nitride-based devices. Therefore, a comprehensive investigation of the crystal quality and surface morphology of AlN films grown on sapphire via MOVPE is of significant importance [3, 4].

In this study, the aim is to investigate the effect of varying Si doping on AlN thin films. For this purpose, AlN films with different Si flow rates were grown on sapphire substrates with MOVPE (Fig. 1). The Si doping levels of the grown AlN films were determined by Secondary Ion Mass Spectrometry (SIMS). X-ray Diffraction (XRD) was used to examine the crystal quality and dislocation densities of the films. The effect of Si doping level on surface properties was investigated through Atomic Force Microscopy (AFM) measurements. In addition, stress analysis of the grown samples was performed with Raman spectroscopy.

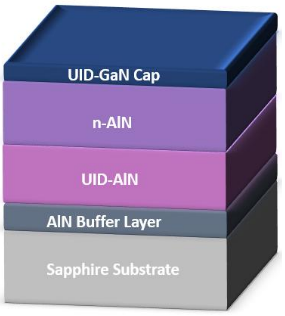

**Fig.1.** Schematic diagram of the MOVPE grown structure on c-plane sapphire substrate.

**Acknowledgments**
The authors acknowledge the usage of the Sivas Cumhuriyet University Nanophotonics Application and Research Center-CÜNAM facilities. This work is supported by the TUBITAK under Project Number 118F425.

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# Superconducting Quantum Interference Devices based on InSb Nanoflag Josephson Junctions

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Keywords: InSb, nanoflags, Josephson junctions, SQUID

In mesoscopic physics, interference effects play a major role in determining the behavior and the transport properties of quantum devices. Superconducting quantum interference devices, known as SQUIDs, are particularly important in applications regarding quantum computing, magnetometry, scanning probe microscopies, and others. Besides, SQUIDs are also used to directly measure fundamental properties of Josephson junctions, like the Current Phase Relationship (CPR).

Here we report the fabrication and characterization of SQUIDs made with InSb nanoflag-based Josephson junctions [1]. These devices are the first DC-SQUIDs realized with two-dimensional nanostructures of InSb [2]. Making use of the elongated shape of the nanoflags, both symmetric and asymmetric SQUID geometries are realized. Characterization at low temperature is performed by magneto-transport measurements, showing supercurrent interference for various values of temperature and back gate.

In the symmetric geometry, the typical SQUID interference pattern is observed. Interference can be controlled by the back gate, which allows to tune from partial to total destructive interference. An additional tuning knob is the applied perpendicular magnetic field, which allows us to choose a working point within the single junction "Fraunhofer" pattern. In the asymmetric geometry, the different response of the two nanoflags to the global back gate leads to the disappearance of interference for certain working points, as shown in Figure 1. SQUID-type oscillations are present at back gate voltage $V_{bg} = 4.5$ V or higher, but not at $V_{bg} = 4.0$ V, where the supercurrent in one Josephson junction has been suppressed.

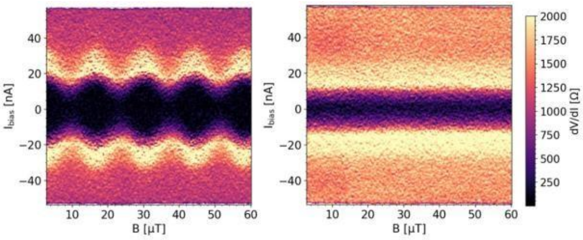

*Fig. 1: Interference pattern of an asymmetric SQUID. Left: at* $V_{bg} = 4.5$ *V. Right: at* $V_{bg} = 4.0$ *V.*

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# Efficient adsorption of $Cd^{2+}$ and $Pb^{2+}$ ions from wastewater using a novel $Fe_3O_4@SiO_2$/PANI-SDBS nanocomposite

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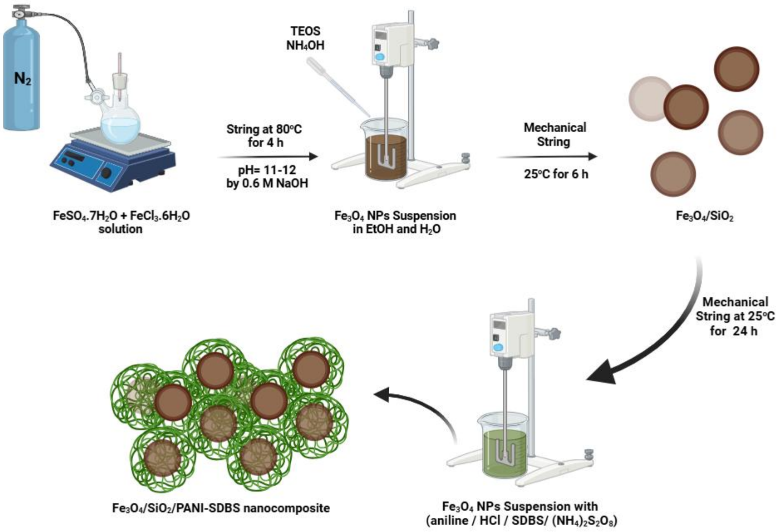
Keywords: Magnetic adsorbents, Surface functionalization, Reusable adsorbents, Adsorption capacity

The current work synthesizes and characterizes a novel $Fe_3O_4@SiO_2$/PANI-SDBS nanocomposite designed as an efficient adsorbent for the removal of $Cd^{2+}$ and $Pb^{2+}$ ions from contaminated water. The process includes the polymerization of aniline on the $Fe_3O_4@SiO_2$ nanocomposite in the presence of SDBS. The $Fe_3O_4@SiO_2$/PANI-SDBS nanocomposite was characterized by using variety of techniques, including FT-IR, XRD, TEM, SEM, BET, TGA, zeta potential measurements, and particle size distribution analysis to evaluate its magnetic, structural, and surface properties. For the elimination of both $Cd^{2+}$ and $Pb^{2+}$ ions, ideal adsorption parameters were examined, including pH, adsorbent dose, and contact duration. The solution medium's optimal pH for achieving the highest effectiveness of elimination for both metal ions was decided to be 7.0. The $Fe_3O_4@SiO_2$/PANI-SDBS adsorbent demonstrated high adsorption capacity due to its large specific surface area and the strong binding affinity of the polyaniline (PANI) and sodium dodecylbenzene sulfonate (SDBS) functional groups for $Cd^{2+}$ and $Pb^{2+}$ ions. Multilayer adsorption on heterogeneous surfaces was shown by isotherm analysis that matched the Freundlich model and adsorption kinetic investigations that showed strong conformance with pseudo-second order for both metal ions. The thermodynamic study proves endothermic and spontaneous process for the removal of metal ions. Furthermore, the adsorbent may be readily recovered from solution thanks to the magnetic core, and regeneration by acid treatment enables reusability with consistent adsorption efficiency across several cycles, making it a cost-effective and sustainable option for continuous water purification processes. Its high adsorption capacity and reusability also make it suitable for use in emergency response situations, such as the rapid cleanup of heavy metal pollution in water.



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# STEM characterization of III-V nanowires using 4D-STEM and Differential Phase Contrast

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Keywords: TEM/STEM. III-V semiconductors.

In recent decades, we have witnessed the development of new analytical tools in the frame of STEM/TEM characterization such as, Differential Phase Contrast (DPC) or 4D-STEM technique, which have changed the paradigm of its uses. The core idea behind DPC is to measure the differential phase shift between two orthogonally polarized beams of light transmitted through a sample. One of the most interested applications in semiconductors is the detection of local electric fields [1]. In 4DSTEM, a highly collimated electron beam scans over the sample, resulting in a diffraction pattern recorded for each scanning position. This creates a dataset that includes information about position (2D) and diffraction pattern (2D), resulting in a 4D dataset. It allows strain calculations or orientation mapping for nanoparticles, among other possibilities [2]. In this work, we present some preliminary results carried out on III-V nanowires as an example to show the potential of these novel techniques. In figure 1 we show DPC data carried out at the surface of the nanowire revealing the existence of a local electric field which can be due to the formation of a core. Figure 2 shows preliminary normal ($\square_{xx}$ and $\square_{yy}$) strain maps carried out on the GaInP section of the nanowire using open scrips [3]. These first results reveal compression ($\square_{xx}$ and $\square_{yy}$ negative) in both x and y direction, being more significant in x-direction. More theoretical work is ongoing to have deeper understanding of the data achieved.

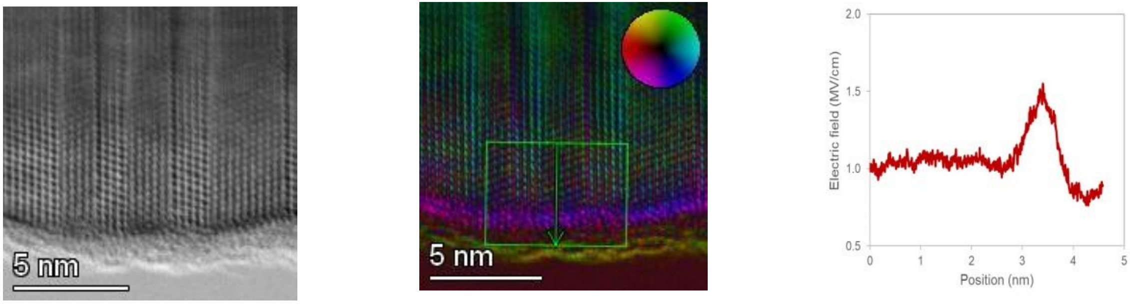

**Fig1:** Electric field detection in III-V nanowire external surface by Differential Phase Contrast (DPC).

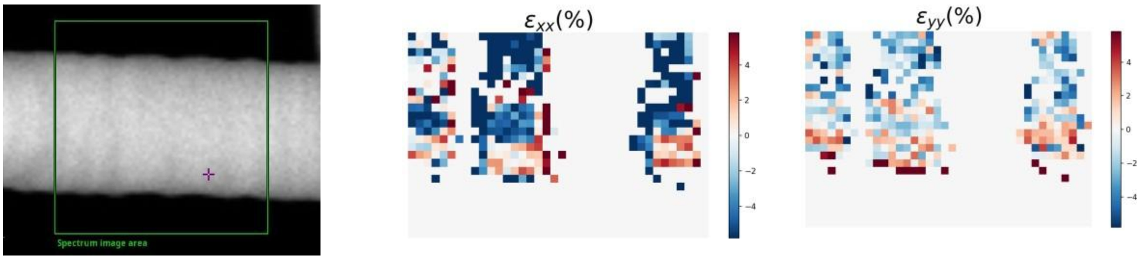

**Fig2:** Normal ($\square_{xx}$ and $\square_{yy}$) strain maps carried out on GaInP region **achieved by 4D-STEM**

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# STM investigation of novel structures of Gallenene intercalated in epitaxial Graphene

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Keywords: Epitaxial Graphene, Gallium, Gallenene, Intercalation, STM, MBE

The development of novel two-dimensional materials is a key focus in the search for nextgeneration functional materials with unique physical and electronic properties [1]. Two-dimensional gallium (gallenene) is an emerging material in the Xenes family [2]. Due to the difficulty in its isolation, there are still few experiments related to its fabrication and the resulting structure. In this work, we fabricate gallenene samples via the intercalation in epitaxial graphene grown on silicon carbide [3, 4]. We investigated the atomic structure of intercalated gallenene using scanning tunneling microscopy (STM), low-energy electron diffraction (LEED), and Raman spectroscopy. Our results reveal the formation of novel gallium structures, including different atomic arrangements and different moiré patterns. To increase our understanding of the formation of these structures, their stability has been monitored along with successive thermal treatments. Our findings highlight several aspects of the atomic structure of the gallium/graphene system shedding a new light on this platform with potential applications in nanoelectronics and quantum technology.

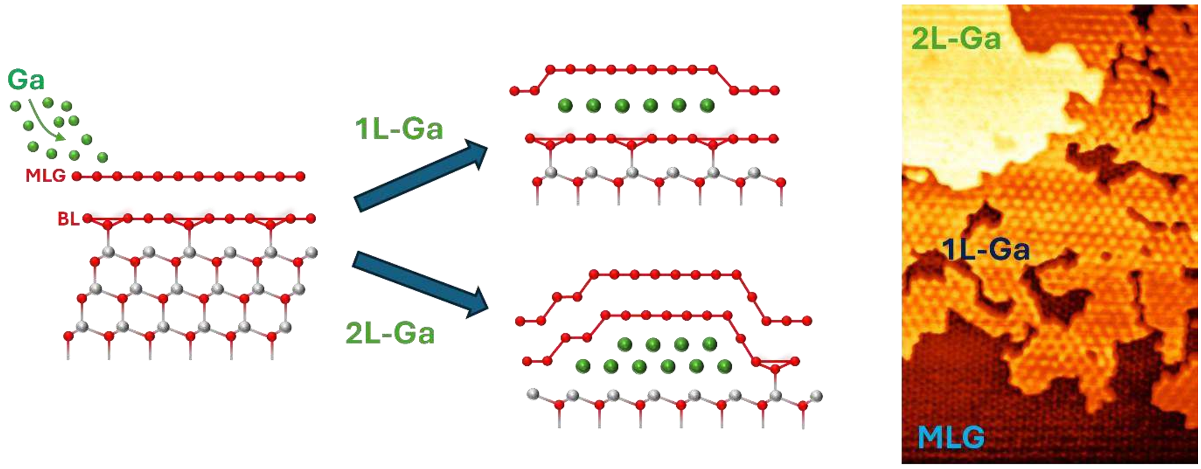

**Fig. 1.** Left: sketch of the Ga deposition on monolayer epitaxial graphene (MLG) and the subsequent intercalation as a single layer gallenene (1L-Ga) and bilayer Ga (2L-Ga). Right: 60x100 nm$^2$ STM image which shows both 1L-Ga and 2L-Ga.

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# *In-situ* TEM investigation of Bi quantum dots formation

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Keywords: in-situ TEM, GaAs, Bi quantum dots

In-situ transmission electron microscopy study of Bi quantum dots (QD) formation in annealed GaAsBi/AlAs multiple quantum well (MQW) structure is presented in this work. The investigated structure, containing two GaAsBi QWs and embedded in AlGaAs parabolic quantum barrier (PQB) was grown on semi-insulating GaAs(100) and was transferred onto an in-situ heating holder (DENS solutions) and heated up to 650 °C. Sample evolution was continuously recorded in-situ in Bright-Field STEM mode. Analysis revealed that QD formation occurs at lower annealing temperatures in case of in-situ heating of lamella than in bulk. In addition, we find that the mechanism governing Bi QD formation is different in the in-situ TEM experiment compared to bulk ex-situ annealing. Comparison of the ex-situ and in-situ annealed structures, as well as in-depth post-annealed structure TEM analysis is presented.

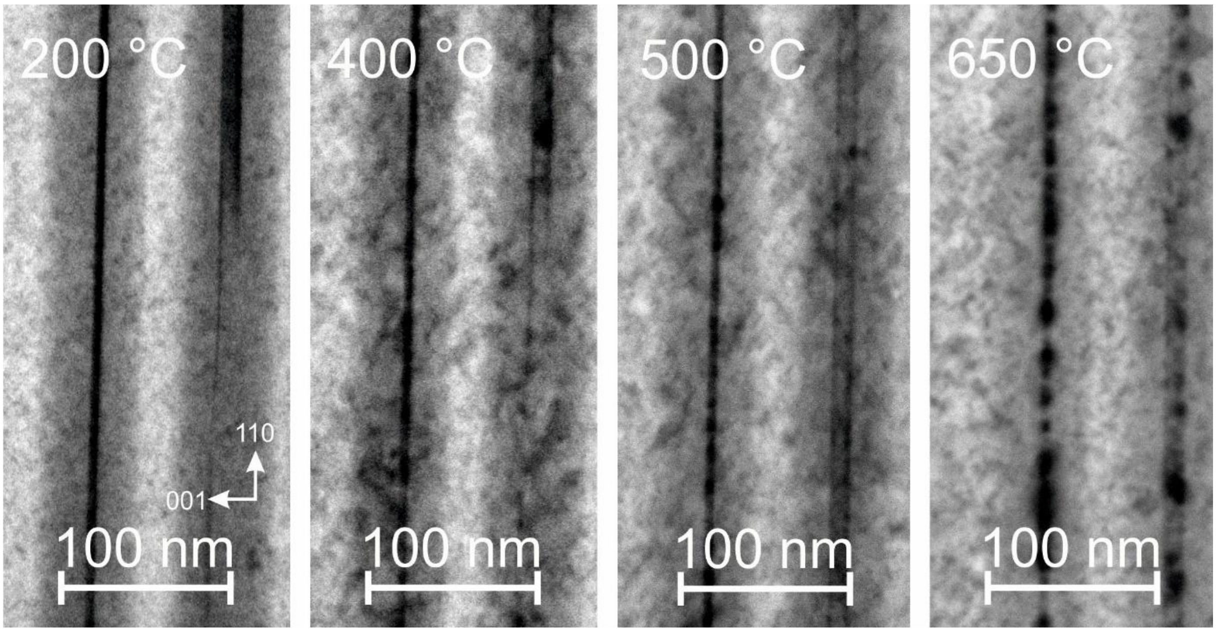

Figure 1. STEM micrographs of sample evolution during heating experiment at temperatures from 200°C up to 650°C. Formation of Bi QDs is visible at temperatures higher than 400°C

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# Real-Time Study of Surface-Guided Nanowire Growth by In Situ Scanning Electron Microscopy

Kristýna Bukvišová*[2,3], Amnon Rothman*[1], Libor Novák[5], Tomáš Šikola[2,3], Ernesto Joselevich^[1], Miroslav Kolíbal*[2,3]

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Keywords: graphoepitaxy, in-plane nanowires, in-situ electron microscopy

Surface-guided growth has proven an efficient approach for the production of nanowire arrays with controlled orientations and their large-scale integration into electronic and optoelectronic devices. Much has been learned about the different mechanisms of guided nanowire growth by epitaxy, graphoepitaxy and artificial epitaxy. Yet, many aspects of the surface-guided growth process remain unclear due to a lack of its observation in real-time.

In this contribution, I will present our observations of surface-guided nanowires growth in real-time by in situ scanning electron microscopy (SEM). Movies of ZnSe surface-guided nanowires growing on periodically faceted substrates of annealed M-plane sapphire clearly show how the nanowires elongate along the substrate nanogrooves while pushing the catalytic Au nanodroplet forward at the tip of the nanowire. The movies reveal the timing between competing processes, such as planar vs nonplanar growth, catalyst-selective vapor-liquid-solid elongation vs nonselective vapor-solid thickening, and the effect of topographic discontinuities of the substrate on the growth direction, leading to formation of kinks and loops. Decrease in precursor concentration as it is consumed after long reaction time, causes the nanowires to shrink back instead of growing, thus indicating that the process is reversible and takes place near equilibrium.

Throughout the presentation, I will demonstrate the power of in-situ microscopy for disentangling the growth mechanisms during epitaxy, and I will also discuss the related instrumentation we developed for the purpose in the past.

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# Heteroepitaxial Growth Modes Revisited

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Keywords: Heteroepitaxy, Growth modes, Nucleation theory

Thin film growth is a fundamental process in materials engineering and it can occur through various mechanisms, including epitaxial growth, meaning that the film is crystallographically oriented to the substrate. Heteroepitaxy is the growth of a film of another material than the substrate, and thus another crystallographic structure. Heteroepitaxy has revolutionized the semiconductor industry, allowing for the integration of materials with different properties into a single device, leading to improved performance and functionality.

It is well known that the outcome of a heteroepitaxial growth experiment is determined by surface and interface energetics, which can be collected in one parameter, the change in surface and interface energy, $\Omega$. It is common knowledge that at equilibrium conditions, $\Omega < 0$ leads to two-dimensional (2D) growth and $\Omega > 0$ leads to the formation of three-dimensional (3D) islands. Using classical nucleation theory, we demonstrate the existence of an interval for the chemical potential difference, $\Delta\mu$, during growth, where 2D nucleation is favorable for sufficiently small, but positive $\Omega$. For larger $\Omega$, 2D nucleation is suppressed in favor of 3D nucleation, see Fig. 1.

We exemplify these results [1] for a couple of cases where epitaxial growth is performed at low supersaturation: vapor–liquid–solid growth of nanowires, and liquid phase epitaxy. First, we explain why certain axial nanowire heterostructures can be grown straight in both interface directions. Second, we explain the formation of multilayer heterostructures in liquid phase epitaxy. Finally, we discuss Stranski–Krastanow growth at low supersaturation and show that there is a thermodynamically defined critical thickness, which increases with the chemical potential difference.

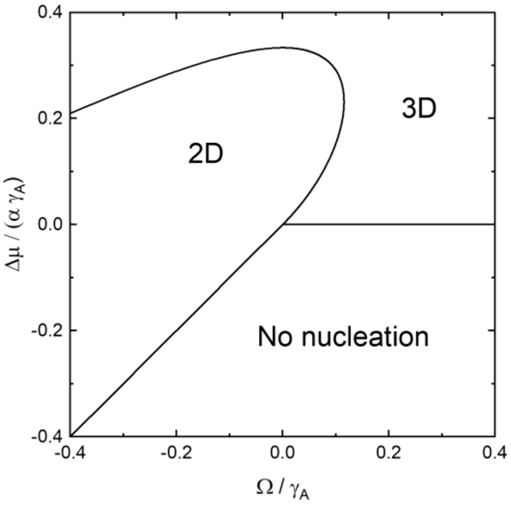

**Fig. 1** The boundaries for 2D, 3D, and no nucleation for hemispherical (3D) and semicircular (2D) nuclei with isotropic surface energy visualized using scaled, dimensionless coordinates, where $\gamma_A$ is the surface energy of the deposited material and $\alpha$ is the molecular volume divided by the height of a monomolecular layer. More details are given in ref. [1].

[1] J. Johansson, *CrystEngComm* **25** (2023) 6671

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# Topotactic Growth of Eu-based Zintl-phase Nanowires and Thin Films by Molecular Beam Epitaxy

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Keywords: MBE, Zintl-Phase, Topotaxy, Antiferromagnetism, Nanowires

Eu-based Zintl compounds have emerged as magnetic topological materials, thanks to the interplay between antiferromagnetic (AFM) order and strong spin-orbit coupling [1]. To harness their exotic electronic states and realize robust boundary modes for quantum devices, precise epitaxial growth methodologies that enable various forms and crystal structures are essential. Here, we pioneer a novel strategy in epitaxial growth: topotaxy [2]. Not only have we successfully grown Zintl-phase $Eu_3In_2As_4$ and $Eu_5In_2As_6$ nanowires (NWs) using molecular beam epitaxy (MBE), but we also extended this method to achieve high-quality $Eu_5In_2As_6$ thin films. Beginning with wurtzite (WZ) InAs and zincblende (ZB) InAsSb NWs grown on InAs substrates, we introduced Eu and As flux, facilitating the migration and exchange of In and Eu atoms within the InAs lattice. This process led to the formation of single-crystal $Eu_3In_2As_4$ and $Eu_5In_2As_6$ grains along the NW cores. Even more remarkably, this growth mechanism enables the formation of Zintl-phase $Eu_5In_2As_6$ thin film directly on InAs substrates. High-resolution transmission electron microscopy (HRTEM) and energy-dispersive X-ray spectroscopy (EDS) analyses confirm atomic-level structural transformations, revealing distinct growth orientations. $Eu_3In_2As_4$ grains align in two orientations relative to the underlying InAs NWs, whereas $Eu_5In_2As_6$ grains extend with three-fold symmetry, growing anisotropically along the *c*-axis of their orthorhombic lattice [3]. Furthermore, $Eu_5In_2As_6$ thin films grown on both InAs (100) and (111)B substrates exhibit preferential *b*-axis alignment, establishing a new frontier for controlled heteroepitaxy. Both NWs and films demonstrate AFM ordering, as confirmed by magnetic susceptibility measurements using a magnetic property measurement system (MPMS) and a scanning superconducting quantum interference device (SQUID). While $Eu_3In_2As_4$ NWs undergo an AFM transition at $\sim$6.5 K, $Eu_5In_2As_6$ NWs and films have two transitions at approximately 5 and 16 K. The ability to selectively convert InAs NWs into different Zintl phases and further extend this growth method to thin films marks a significant advancement in epitaxial engineering. This versatile topotactic growth approach unlocks new opportunities for quantum computation and spintronic applications.

## Reference

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# Van der Waals Epitaxy and Characterization of Quasi Two-Dimensional Ge-Sb-Te Materials

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Keywords: phase-change materials, ferroelectricity, molecular beam epitaxy (MBE)

The emergence of two-dimensional materials has significantly expanded the scope of materials science over the past decade, offering promising breakthroughs across various technological domains. Among the different synthesis methods, van der Waals (vdW) epitaxy stands out for its ability to provide high quality, purity, and scalability, essential factors for seamless integration with microelectronics.

Chalcogenide phase-change materials (PCMs) are recognized as strong candidates for the development of storage-class memory devices and brain-inspired computing. (PCMs) operate based on their ability to switch between two or more distinct phases, typically an amorphous (disordered) and a crystalline (ordered) state, in response to external stimuli such as heat, electric current, or light. This transformation is reversible, making PCMs suitable for non-volatile memory applications. The most widely used material for memory applications is Ge-Sb-Te alloys, particularly the $Ge_2Sb_2Te_5$ (GST) compound. GST is commonly employed in PCM memory devices due to its excellent switching performance, fast transition times, and good retention characteristics.

Beyond their well-known application in non-volatile memory, the Ge-Sb-Te family of materials exhibits a range of unique properties. For example, GeTe, a binary compound, is the foundation of a new class of materials called ferroelectric Rashba semiconductors, where ferroelectricity is leveraged to control spin texture at room temperature. A key factor in harnessing these diverse properties is achieving high crystal quality and interface control, both of which are facilitated by molecular beam epitaxy (MBE) for material deposition.

In this presentation, I will begin by providing an overview of the MBE fabrication process for Ge-Sb-Te layered materials and heterostructures on Sb-passivated Si(111) substrates. I will then discuss the vdW epitaxy and characterization of GeTe-rich $(GeTe)_m(Sb_2Te_3)_n$ (GST) films, which have recently shown breakthrough results indicating composition-dependent ferroelectric behavior.[1]

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# PLD-based integration of strontium titanate thin films with silicon substrate for robust solar water splitting

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Keywords: silicon, strontium titanate, pulsed laser deposition, epitaxy, photocathode, water splitting

Development of a robust photocathode using low-cost and high-performing materials, e.g., p-Si, to produce hydrogen has remained challenging since the silicon substrate is easily susceptible to (photo)corrosion under photoelectrochemical (PEC) operational conditions. A protective layer over the substrate to simultaneously provide corrosion resistance and maintain efficient charge transfer across the device is therefore needed. In the present work we will focus on different approaches used for functionalization of silicon surface with the aim of (epitaxial) integration high-quality $SrTiO_3$ (STO) layer to passivate the p-Si substrate. We will showcase different surface terminations as well as application of reduced graphene oxide (rGO) buffer layer as key steps in successful integration of STO with p-Si. Additionally, the role of STO thickness, its crystalline and interfacial quality in contact with p-Si on PEC hydrogen evolution will be assessed. Finaly, we will highlight most viable routes for preparing a robust protection layer over a p-Si photoelectrode substrate in realizing an efficient and, at the same time, durable PEC device.

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# SiGe:B Source/Drain epitaxy for advanced device applications

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**Keywords**: Source/Drain, group IV, epitaxy, nanosheet, CFET, CMOS

Nanosheet (NS) and complementary field-effect transistors (CFET) [1] are now considered as main device architectures for CMOS technology nodes beyond 2 nm, where SiGe:B and Si:P epitaxial layers are typically used as p- and n-type source/drain (S/D) layers, respectively. Due to their high aspect ratios and densities, such scaled devices introduce many challenges to maintain acceptably low access resistances [2]. This work presents progress in SiGe:B epitaxy for NS and monolithic CFET (mCFET) devices (Fig. 1.a). It includes systematic epitaxy studies on the different surface orientations existing in devices (Fig. 1.b-e).

S/D epitaxial layers were grown by chemical vapor deposition (CVD) on 300 mm blanket and patterned Si wafers, using conventional and low-temperature (LT) processes (≤ 500°C). For nonselective conventional processes, the highest active boron concentrations ($[B]_{act}$) were obtained on Si(111) substrates (Fig. 1.f). On Si(001), the $[B]_{act}$ is limited to ~ $1\times10^{21}$ $cm^{-3}$ and dropped by a factor 2 after the recovery of the selectivity with respect to the dielectrics. On patterned wafers, LT processes showed promising performance improvements, with $[B]_{act} > 1\times10^{21}$ $at.cm^{-3}$, while maintaining the full process selectivity. These values were estimated assuming a Hall scattering factor of 1.

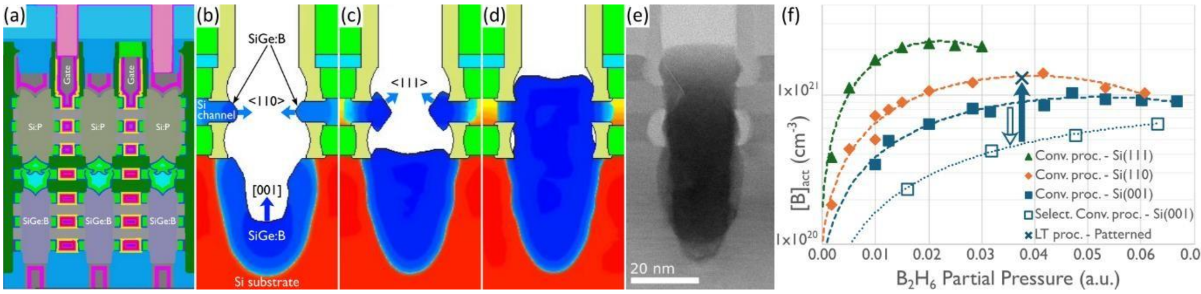

***Figure 1****: Schematic of (a) a generic mCFET structure, (b)-(d) predicted nucleation and evolution of the SiGe:B S/D epilayers in a NS device structure,(e) BF-STEM image of a typical SiGe:B S/D epilayer obtained with conventional process. (f) Active boron concentration as a function of $B_2H_6$ partial pressure used during the growth of SiGe:B on blanket with different surface orientation using conventional processes, and on patterned wafers using LT process. Blue arrows show the variation in active boron concentration induced by selective (hollow arrow) and LT (full arrow) processes.*

[1] *S. Demuynck et al., VLSI 2024*
[2] *P. Raghavan et al., IEEE CICC 2015*
[3] *This work has been enabled in part by the NanoIC pilot line. The acquisition and operation are jointly funded by the Chips Joint Undertaking, through the European Union's Digital Europe (101183266) and Horizon Europe programs (101183277), as well as by the participating states Belgium (Flanders), France, Germany, Finland, Ireland and Romania. For more information, visit nanoic-project.eu. The imec core CMOS program members, local authorities and the imec pilot line are acknowledged for their support. A. P. acknowledges FWO for the Strategic Basic Research PhD fellowship grant 1S20225N.*

# Manipulating Electronic and Magnetic Properties of a 2D Antiferromagnetic Material through Interface Effects

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Keywords: 2D material, structural and electronic properties manipulation, interface effects

Recent developments in 2D magnetism have led to the search for novel van-der Waals intrinsic magnetic materials to explore new magnetic phenomena in the 2D limit. Transition metal phosphorus trichalcogenides are two-dimensional (2D) van der Waals semiconductors that have in the most cases an intrinsic antiferromagnetic ordering. These materials have potential applications in electronics, optoelectronics, spintronics, and magnonics. The electronic and the spin structure of these materials strongly depend on the transition metal elements. Herein, we present the studies of properties of nickel phosphorus trisulfide (NiPS3) at the interface with a very thin film of Co in the coverage range from sub-monolayer to 3 monolayers, using synchrotron-based techniques. In-situ measurements of the structure using low energy electron diffraction, microscopy and photoemission microscopy and spectroscopy (LEED/LEEM and XPEEM, XPS) combined with X-ray absorption spectroscopy (XAS) with x-ray linear and circular magnetic dichroism (XMLD and XMCD) and angle-resolved photoemission (ARPES) with linearly polarized beams was utilized to directly probe growth mode, chemical and magnetic state, as well as the momentum-resolved electronic structure. The systematic investigation of the induced changes by the cobalt deposition and their effects on the structural and electronic properties of the NiPS3 system is essential not only for understanding the mechanism of low-dimensional magnetism but also for designing the next generation of low-cost and low-power consumption electronic and spintronic devices.

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# Cost-effective solar water splitting with III-V/Si epitaxial photoelectrodes

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Keywords: photo-electrochemistry; electrolysis; catalysis; III-V semiconductors; silicon

In this contribution, we report on the recent achievement of epitaxial III-V/Si photoelectrodes for solar hydrogen production. After having recalled the motivation for producing hydrogen from renewable energies, [1-4] the basic concepts of electrochemistry will be first introduced, including overpotentials, catalysis and associated challenges. The physics of photoelectrochemical cells will then be explained, and the interest of using epitaxy for bandgap and band lineup engineering and doping control will be highlighted. [5-8] Finally, results obtained about the characterization of III-V/Si photoelectrodes using Pt, Ni or $MoS_2$ catalysts, will be discussed in terms of stability, performance and cost.[9]

The authors acknowledge RENATECH (French Network of Major Technology Centers) within Nanorennes and C2N-PANAM platform for technological support. This research was supported by the “France 2030” program of the French National Research Agency, NAUTILUS Project (Grant no. ANR-22-PEHY-0013), the EQUIPEX NANOFUTUR (ANR-21-ESRE-0012), Rennes Métropole and Région Bretagne.

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# High-photocatalytic activity of PA-MBE grown GaN nanowires for degradation of methylene blue

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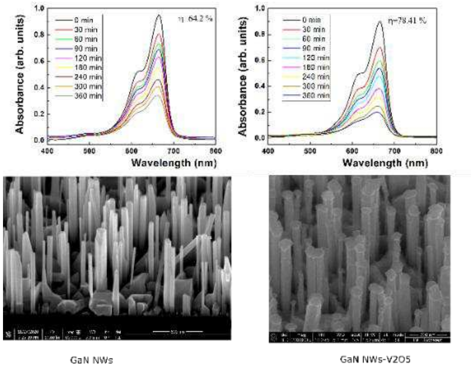
Keywords: GaN nanowires; molecular beam epitaxy; photocatalysis.

Various efforts have been undertaken to develop efficient, environmentally friendly, and low-cost methods for removing organic dyes/pollutants from the water with reduced energy consumption [1,2]. Gallium nitride (GaN) and related materials synthesized by plasma assisted molecular beam epitaxy (PA-MBE) under nanowire (NW) form with sub-100 nm diameter appear as good photocatalysts candidate. Despite its wide band gap, which can appear as a drawback for photocatalytic decay under sunlight, GaN presents a high flat-band potential (approximately equal to conduction band edge for n-type conductors of -1.5 eV). This is unambiguously advantageous because the photogenerated electrons in the conduction band must have high reduction potential. In addition, the large surface-to-volume ratio of the nanowires increases the usable conversion area in the photocatalytic decay[3]. Finally, GaN is characterized by very high chemical, thermal and ionizing radiation stability in comparison with the most widely used materials, such as the metal oxides. This confers a given reproducibility during photocatalysis cycles, a longer life time, and thus offers a better reusability, even in hostile environments with low and high pH values.



GaN NWs

GaN NWs-V2O5

*Figure 1: UV–Vis absorption spectra for the photodegradation of MB dye at different irradiation times in the presence of GaN NWs and GaN NWs/$V_2O_5$ heterostructures.*

In this work, we investigate the relationship between the GaN NW morphology and their photocatalytic activity for degradation of the methylene blue at different pH values. By adjusting the growth temperature of the PA-MBE growth GaN NW, we have modulated their morphology, going from GaN NWs surrounded at their bottom with a rough 2D-layer, giving rise to an additional layer at the interface of Si-GaN NWs, to GaN NWs directly connected to the Si-substrate. In order to push our investigation and analyse the ability of GaN NWs to work in harsh environments, we have examined the NW presenting the best photocatalyst performances under extreme acidic (pH = 2.3) and alkaline conditions (pH = 10). Moreover, heterostructures with enhanced absorption in the visible range of the electromagnetic spectrum, such as InGaN/GaN and $V_2O_5$/GaN heterostructures (Figure 1) are proposed in order to enhance the photocatalytic activity of GaN NWs under sunlight.

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S10.02

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# Investigating the Oxidation/Reduction Mechanism of Zinc Phosphide by In-Situ Transmission Electron Microscopy

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Keywords: Oxidation, Reduction, Zinc Phosphide, Environmental TEM

The proposed oral presentation will revolve around the research I carried out during my stay at the NanoLund laboratories at the University of Lund within the OPERA-STSM framework. In the month I was there, I investigated the reduction/oxidation mechanism of Zn3P2 nanowires via in-situ observation in the HITACHI 300kV ETEM. Zn3P2 instantly develops a thin oxide layer as soon as it is exposed to air, leading to the worsening of its properties for PV applications. Although unwanted, this feature is rather unavoidable when the material is grown ex-situ in the MOCVD chamber and later moved outside for further processing within the solar cell fabrication chain. The first part of the investigation dealt with the deep understanding of the native oxide in terms of thickness, crystallinity and elemental composition. To fulfill this task the HITACHI microscope was operated in transmission mode without any gas injection in the beam column. Once we assessed the nature of the native oxide, we moved to the reduction of oxide to recover the pristine Zn3P2 surface. The chamber of the in-situ TEM was filled with Phosphine (PH3) to create a reductive environment for the oxide shell. Different partial pressures and temperature were investigated to achieve the objective. Unfortunately, all the trials resulted in the same observation: once both the temperature and PH3 partial pressure were high enough for the reaction to happen, the Zn3P2 core was the first to be attacked leaving behind the unaltered oxide shell. Further compositional characterization proved that indeed the oxide was altered: from a Zn rich phase (ZnOx), the residual oxide was mainly composed of P and O. The study that I carried out highlighted the difficulty in getting rid of the unwanted oxide during the fabrication process, making it essential to find other strategies to mitigate the problem.

Funded by the European Union

# Tunable $GaAs_xP_{1-x}$ Quantum-Dot Emission in Wurtzite GaP Nanowires

Robert Andrei Sorodoc[1] , Paolo De Vincenzi[2], Akant Sagar Sharma[2], Giada Bucci[1*], Mario Roggi[2], Enrico Mugnaioli[3], Lucia Sorba[1], Marta De Luca[2], and Valentina Zannier[1]

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Keywords: Nanowires, Quantum Dot, Chemical Beam Epitaxy, Photonics

Quantum light emitters can be realized by employing semiconductor quantum-dots (QD) for advanced quantum optics and nanophotonic applications. Tunable Gallium Arsenide Phosphide ($GaAs_xP_{1-x}$) QD in nanowires (NWs) with emission in VIS-NIR wavelength range have a strong technological potential. Here, we synthesized crystal-pure wurtzite Gallium Phosphide (GaP) nanowires (NWs), incorporating single $GaAs_xP_{1-x}$ QDs of various As content with a great degree of control over the shape and composition of the ternary alloy QD. A well-defined confinement of the QD and the tunability of the emission wavelength are confirmed by low-temperature micro-photoluminescence (µ-PL) spectroscopy showing that the QD NW emission is dominated by a narrow peak whose energy shifts according to the As content of the QD (Fig. 1). Moreover, a localized and efficient carrier recombination mechanism is found by single-NW µ-PL mapping, confirming that this emission arises from the QD. Finally, a power and temperature dependent µ-PL study is performed to characterize the QD excitonic properties and to identify the origins and the nature of the involved energy levels [1].

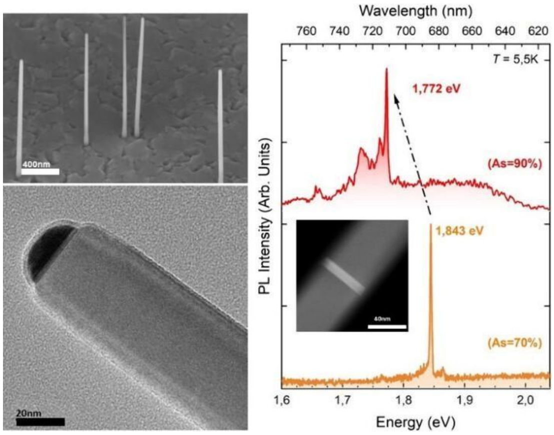

**Fig.1** Scanning and transmission electron microscopy images (left side panels) and low-temperature µPL spectra (right side panel) of $GaAs_xP_{1-x}$ QD NWs with As = 70% and As = 90%.

[1] Robert Andrei Sorodoc, Paolo De Vincenzi, Akant Sagar Sharma,, Giada Bucci, Mario Roggi, Enrico Mugnaioli, Lucia Sorba, Marta De Luca, and Valentina Zannier, Tunable GaAsxP1–x Quantum-Dot Emission in Wurtzite GaP Nanowires, ACS Applied Materials & Interfaces, in press
DOI 10.1021/acsami.4c15343

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S11.02

# Colossal magnetoresistance at room temperature of manganese-based perovskite epilayers grown on 001 SrTiO3 substrates

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

Several manganites possess large RT-CMR and considering that the highest CMR (Colossal magnetoResistance) occurs at $T_C$, manganites with $T_C$ as close as to RT should be envisaged and engineered for potential room temperature applications. $La_{.67}Ba_{0.33}MnO_3$ (LBMO) has a $T_C$~343K, 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 Å, favoring the epitaxial growth on the SrTiO3 (STO) 100 surface, due to extremely low lattice mismatch (aSTO = 3.905 Å). Doping with Ti (2%), the lattice constant of La.67Ba.33Ti.02Mn.98O3 (LBTMO) increases to 3.912 Å, 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 Å. 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 ($T^t_C$~295K) or as the extreme value found by representing the temperature dependence of the magnetization derivative ($T^d_C$~286K). 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 TC, 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 eg states of lowest energy. Colossal 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 know on such oxides.

# Optical Properties of Nitrogen-Doped Carbon Quantum Dots

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Keywords: carbon nanoparticles; photoluminescence

Carbon quantum dots (CQDs), fluorescence quasi-spherical nanoparticles with crystalline graphitic core [1], can be synthesized by many methods. Their optical properties were explained by the band gap governed by the size of the $sp^2$-domain (the extent of the π-electron system) [2,3] and surface defects controlled by edge configuration and functional groups, such as hydroxyl, amide, carbonyl, and carboxyl moieties [3,4]. However, the optical properties of solvothermal-synthesized CDs could also be affected by the presence of unreacted species or small organic molecules [5], and the intense excitation-independent photoluminescence (PL) of CDs was indeed attributed to molecular fluorophores, which may be surface-bound or embedded in the CD matrix [6].

Previously, we prepared the nitrogen-doped CQDs (N-CQDs) from glucose and ethylenediamine using a one-step and fast (a few minutes) microwave-assisted hydrothermal synthesis [7]. The average size of the particles was 3.8 nm, and high-resolution TEM confirmed their crystalline graphitic nature. The carbon structure contained 18.6 at.% of nitrogen and 12.6 at.% of oxygen. Later, we observed the spontaneous room-temperature formation of N-CQDs from the same reactants, glucose and ethylenediamine. After 5 months, the spontaneously formed N-CQDs exhibited similar structural properties, optical absorption in the UV-VIS range, and PL emission as those synthesized in the microwave reactor [8].

In this work, we will compare the optical properties of the two above-mentioned N-CQDs with the nanoparticles obtained from plasma-deposited amorphous organic thin films with amino groups. Thanks to these films' partial water solubility, the presence of fluorescent nanoparticles was detected as the fluorescence of water extracts. High-resolution transmission electron microscopy proved that the nanoparticles are graphitic, and their PL spectra also exhibited excitation-dependent emission.

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# Optical properties and electronic structure of zinc-blende $In_xAs_{1-x}P/InP$ quantum dots in nanowires emitting at telecom wavelengths

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Keywords: quantum dots in nanowires, InP-based material system, vapour-liquid-solid chemical beam epitaxy, optical properties and electronic structure

Quantum dots in nanowires (QD-NWs) have been proven a beneficial platform for single-photon sources making use of dielectric screening effect to provide directional emission into a Gaussian mode in the far field [1]. This addresses two important challenges in non-classical light sources – photon extraction efficiency and efficient coupling into single mode fibers. Another advantage of QD-NWs is a possibility to create systems of multiple vertically coupled QD with independently controllable height of each QD, which seems ideally suited for generation of 2D cluster states [2] for a scalable photonic universal quantum computation platform.

This contribution provides an overview of properties of InAsP QDs in zinc blende InP NWs grown by Au-assisted vapour-liquid-solid mode within chemical beam epitaxy technique [3]. It has been demonstrated that the growth can be optimized for high structural quality vertical NWs, together with low spatial NW density facilitating single QD study. Arsenic content in the QD can be tuned in a broad range from 20% up to pure InAs. This translates into shifting the emission wavelength from below 1 μm, through the II and III telecomm windows. An additional degree of freedom is the height of the QD, which allows for fine tuning of the electronic structure of the QD. The electronic structure and resulting optical properties have been modeled using both the tight binding and the 8 band **k·p** method, combined with the configuration interaction approach for excitonic calculations. Photonic properties, like far field emission pattern and photon extraction efficiency, have been first optimized numerically using finite difference time domain technique [4] to provide design input for the QD-NW fabrication and then compared to experimental results obtained by means of optical spectroscopy methods. Eventually, current status and outlook, with emphasis on remaining challenges, will be presented.

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# Mechanism of Ge Quantum Cones Formation by Laser Radiation on a Surface of SiGe/Si Solid Solution Grown by Molecular Beam Epitaxy

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Nanostructures (NSs) are the most studied objects in solid-state physics, especially the quantum confinement effect in systems of quantum dots—0D, quantum wires—1D, and quantum wells—2D. Thanks to these conditions, it is possible to create new electronic and optical devices. It is well known more methods of such structures formed on semiconductor surfaces by widely used methods such as Molecular beam epitaxy (MBE) [1], Ion implantation [2], Chemical vapor deposition [3], Sol-gel [4], Spray [5] and Laser ablation [6] but all these methods uncontrollable. Therefore, the aim of this study is to elaborate the laser method for Ge nanocones formation on a surface of SiGe solid solution grown on Si using MBE with controllable height. In experiment SiGe solid solution with concentration of Ge atoms 30% grown on Si wafer by MBE method was used. The thickness of the solid solution was 200 nm. Pulsed Nd:YAG laser with λ=1.06 µm, pulse duration 15ns, power P=1MW, and diameter of beam 3 mm as a source of light was used. Irradiation of the samples at room temperature, atmospheric pressure, and 70% humidity in scanning mode takes place. Using an Atomic force microscope, it was found that the height of cones depends on the laser intensity: at laser intensity, $I_1$= 2.0 MW/cm$^2$, height is 5.5 nm at $I_2$=7.0 MW/cm$^2$ - 11 nm, and $I_3$=20.0 MW/cm$^2$ - 27 nm. The region of the photoluminescence specter is from 1.2 eV to 2.2 eV, and the maximum is shifted to more than 1 eV - "blue shift" takes place. The mechanism of quantum cones formation on the irradiated surface of SiGe solid solution is characterized by two stages – laser redistribution of atoms and selective laser annealing. The first stage is characterized by the formation of Ge/Si heterostructures due to the drift of Ge atoms toward the irradiated surface of the sample in the gradient of temperature, the so-called Thermogradient effect (TGE) [7]. A New Ge phase is formed at the end of the process. Ge atoms are localized at the surface of Si like a thin film. The heterostructure is characterized by compressive stress of the Ge layer. The second stage is characterized by the formation of nanocones on the irradiated surface of a semiconductor by selective laser annealing of the top Ge layer with following mechanical plastic deformation of the layer as a result of relaxation of the mechanical compressive stress arising between these layers due to mismatch of their crystal lattices and selective laser heating of Ge layer. Evidence of our suggestion is the appearance of the Ge-Ge LO phonon line in Raman spectra.

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# Comparative Study of $VS_2$ Epitaxy on Strained and Relaxed Graphene

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Keywords: STM, Vanadium disulfide, Strain, 2D materials, Graphene

Among transition metal dichalcogenides, $VS_2$ has attracted substantial interest due to its theoretically predicted magnetic and electronically correlated ground states when reduced to a single layer. However, when synthesized on Au(111) [1] and gr/Ir(111) [2], no net magnetic moment has been observed. Consequently, it is widely accepted that the theoretically predicted ferromagnetic ground state is not realized in pristine single layers [2].

Alternatively, the ground state of pristine $VS_2$ could be tuned by modifying the system's subtle interactions, with strain being a common strategy. In this work, we grow $VS_2$ via electron beam epitaxy and characterize it via a variable temperature STM on two different substrates: first, on gr/Ir(111) as a control sample [2], and second, on strained graphene, gr/Ir(332). Graphene experiences strain and compression when grown on a vicinal surface like Ir(332), depending on whether it is located on atomic terraces or stepped areas of the sample [3].

We observe that $VS_2$ grows epitaxially across both areas, exhibiting island bending (panel a). Additionally, the previously reported charge density wave (panel b) is modulated by an additional superstructure resulting from the interaction with the step edges of Ir(332). We demonstrate that straining $VS_2$ by growing it on a vicinal Ir(332) crystal is a promising approach that could open new avenues for modifying the ground-state properties of pristine $VS_2$.

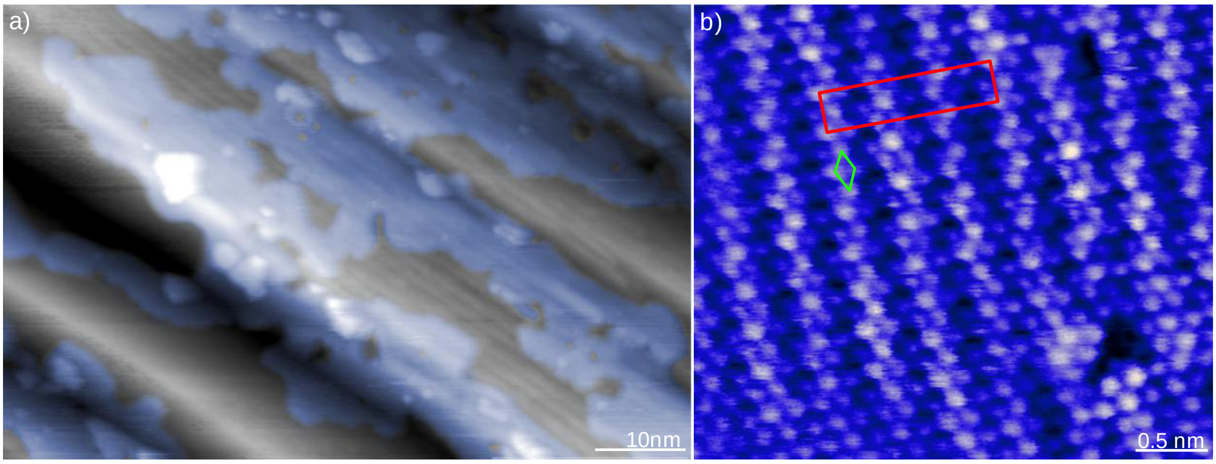

**Figure: $VS_2$-gr/Ir(332).** ***a)*** *STM image of $VS_2$ single layer islands, highlighted in blue, bending over the stepped areas of the gr/Ir(332) sample. Image parameters: V=750 mV, I=800 pA.* ***b)*** *Atomic resolution and charge density wave (CDW) periodicities observed over the surface of a $VS_2$ single layer island, the unit cells are highlighted in green and red respectively. Image parameters: V=5 mV, I=3.2 nA. T=RT.*

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# Tunable Superconducting Transport in 2D-InSb/Nb-based Hybrid Josephson Junctions with Dual-Gate Electrostatic Control

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Keywords: InSb, nanoflags, Josephson junctions

Gate-tunable hybrid Josephson junctions provide a versatile platform for controlling superconducting transport, offering new opportunities for scalable quantum computing and superconducting logic applications. Here, we investigate dual gate electrostatic control on superconducting transport in 2D-InSb/Nb-based hybrid Josephson junction. We fabricate Josephson junctions on 2D-InSb nanoflags with the focus on top gate and bottom gate tunable supercurrent modulation. InSb nanoflags were grown using Au-assisted chemical beam epitaxy (CBE) on InP(111)B substrates [1]. A 300 nm thermally grown $SiO_2$ and 30 nm $HfO_2$ by atomic layer deposition are used as bottom and top gate dielectrics, respectively. The device, characterized at cryogenic temperatures (300 mK), exhibits clear multiple Andreev reflections (MAR) under varying voltage bias and gate control, indicating high junction transparency. Electrostatic gating via back gate voltage (varied between ±40 V) and top gate voltage (varied between ±4 V) demonstrates a clear modulation in the channel conductance, as shown in Fig.1. Systematic magnetic field sweeps from 0 to ±20 mT, at fixed back gate and top gate voltages, result in Fraunhofer patterns. As the back gate increases from 0V to 40 V, the central lobe increases in amplitude, indicating an increase in the Josephson critical current, while the side lobes become more defined, suggesting higher coherence of supercurrent. Our results demonstrate an optimized experimental framework for engineering gate-controlled hybrid superconducting systems, relevant for quantum information processing and next-generation superconducting quantum circuits.

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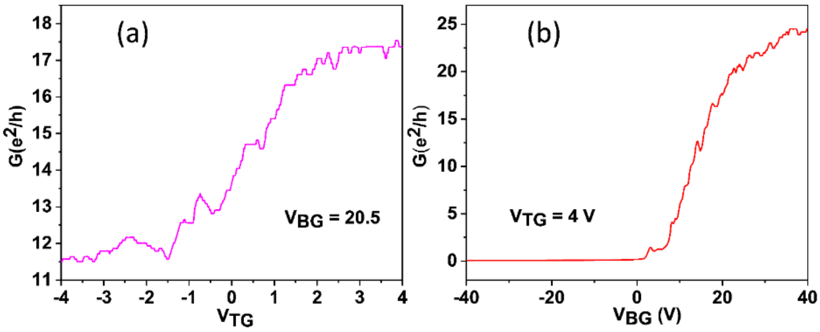

Figure1. Conductance modulation in a dual-gated 2D-InSb/Nb-based hybrid Josephson junction: (a) Conductance vs. top gate voltage at a fixed bottom gate voltage of 20.5 V, and (b) conductance vs. bottom gate voltage at a fixed top gate voltage of 4 V, at T = 4 K.

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# Energy storage properties in ferroelectric epitaxial La:$HfO_2$ based thin film capacitors

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Keywords: Epitaxial hafnium oxide films; Ferroelectric; Energy storage capacitors

Ferroelectric and anti-ferroelectric hafnium oxide are being the point of attraction for developing next-generation energy storage capacitors since they show high energy storage density (ESD), high power density and high efficiency ($\eta$) and are scalable down to the ultrathin limit [1]. Most research on the energy storage performance focuses on the antiferroelectric hafnium oxide, while ferroelectric hafnium oxide has been seldom investigated [1,2]. In this talk, I will show the enhancement of the energy storage characteristics of epitaxial ferroelectric orthorhombic lanthanum-doped hafnium oxide-based 2D capacitors by introducing a thin dielectric amorphous alumina capping layer. It is revealed that the inclusion of a dielectric layer influence both the ESD and $\eta$ of the fabricated capacitors due to the depolarizing effect increase as a result of the presence of the alumina layer. These results shine light on the potential use of epitaxial ferroelectric $HfO_2$-based capacitors for highperformance energy storage applications.

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# Mechanisms of Meander Formation: The Role of Surface Energy Potential

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Keywords: cellular automaton, crystal surface, diffusion

In the fabrication of electronic and optoelectronic devices, surface morphology and its evolution during crystal growth are of crucial importance. Achieving control over surface growth to obtain a desired surface pattern is a key goal, but, this control is challenging due to surface instability, as even small energy barriers can have significant effects. One of the primary instabilities is step meandering, a morphological instability driven by surface diffusion.

We investigated the role of the surface potential energy landscape in meander formation using the (2+1)D Vicinal Cellular Automaton model[1]. By distinguishing surface diffusion from adatom incorporation, we isolated key factors influencing surface pattern dynamics. A detailed analysis of the diffusion process revealed that modifications to the potential energy well and the barrier at the top of the step significantly impact meandering. Results demonstrate that the presence of a potential well at the bottom of the step alone is sufficient to induce meander formation. Additionally, we examined the influence of the Ehrlich-Schwoebel barrier on meander evolution and proposed mechanism for meander formation. These findings highlight the fundamental role of surface energy potential in shaping surface morphology, offering new insights into the mechanisms governing pattern formation.

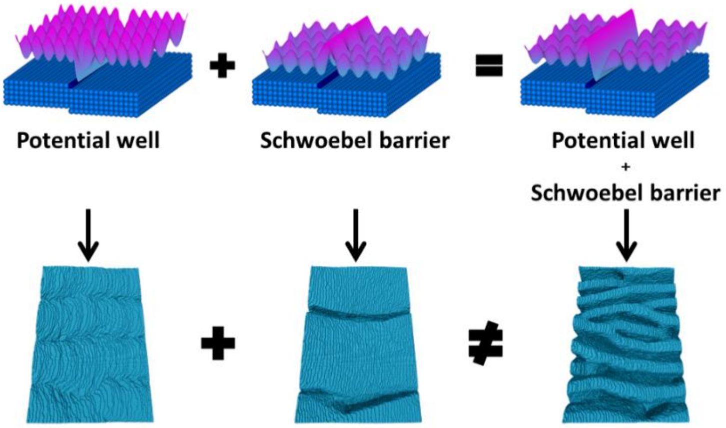

Fig. 1. Meanders and corresponding potential shape obtained in the presence only of the potential well, only of the Ehrlich-Schwoebel barrier and in the presence of both potentials.

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# Engineering relaxor ferroelectric epitaxial thin films for low voltage energy storage applications

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Keywords: Epitaxial relaxor ferroelectric; energy storage; relaxor behavior; polar nanoregions

In this work, we engineered the morphology of lead-free 0.85[0.6Ba(Zr$_{0.2}$Ti$_{0.8}$)O$_3$-0.4(Ba$_{0.7}$Ca$_{0.3}$)TiO$_3$]-0.15SrTiO$_3$ (BZCT-STO) epitaxial thin films, fabricated by the pulsed laser deposition technique. The annealing time changes both the grain shape and size that were found to control the relaxor behavior of the BZCT-STO films. The enhanced relaxor behavior, assigned to the formation of polar nanoregions, was achieved in the film with uniform smaller spherical grains. The electric field dependence on the ferroelectric and energy storage properties of the BZCT-STO thin films, annealed at different times, is investigated. It is found that the LSMO/BZCT-STO/Au capacitor with the enhanced relaxor behavior shows the optimum energy storage performance attributable to a moderate maximum polarization and remnant polarization difference, and the highest electric breakdown field. An energy storage density of 9.24 J/cm$^3$, with an efficiency of 86.4%, at an applied electric field of 1500 kV/cm, was obtained. The elevated energy storage density and efficiency in these epitaxial BZCT-STO thin film capacitors make them one of the most promising systems reported in the literature for energy storage applications at low applied electric fields/voltages.

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# Resistive switching in 2D $MoO_3$ studied by atomic force microscopy

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Keywords: epitaxial molybdenum trioxide, 2D oxide, resistive switching, atomic force microscopy

Since the discovery of graphene, two-dimensional (2D) van der Waals (vdW) layered materials have gained significant attention due to their exceptional electrical and optoelectronic properties. These materials have found applications in a variety of fields, ranging from flexible electronics to photonics. Recently, there has been growing interest in their potential for data storage applications, particularly in resistive random access memory (ReRAM) and neuromorphic computing. The operation of these memory devices relies on the resistive switching (RS) phenomenon, which enables the reversible change of resistance states in a material under electrical stimulation.

Although extensive research has been conducted on the global characterisation of metal-insulator-metal (MIM) structures in RS-based devices, localised studies at the nanoscale have not been explored. In this work, we present investigations of resistive switching in a two-dimensional transition-metal oxide using atomic force microscopy (AFM). Specifically, we studied epitaxially grown molybdenum trioxide ($MoO_3$) films deposited by thermal evaporation under ultra-high vacuum conditions onto highly oriented pyrolytic graphite (HOPG). The chemical composition was investigated by X-ray photoelectron spectroscopy (XPS). The analysis revealed a slight nonstoichiometry in monolayer samples, while thicker films showed more stoichiometry. Using AFM-based conductive measurements, we demonstrated bipolar resistive switching, with the SET process occurring under negative voltage polarisation, and the RESET process taking place under positive voltage polarisation. Additionally, we observed degradation of the material induced by electrostimulation. These results highlight the potential of 2D transition metal oxides for next-generation memory technologies and underscore the importance of nanoscale characterisation in understanding resistive switching mechanisms.

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# Engineering Strain in 2D Materials: Surface Interactions and Substrate Modification

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Keywords: 2D materials, MBE, strain, screening, substrate interactions, band gap change

Two-dimensional (2D) materials, particularly transition metal dichalcogenides (TMDs), exhibit remarkable properties such as 2D superconductivity, magnetism, tunable bandgaps, and correlated states. The ability to modify their band structure via functionalization, substrate interaction, heterostructures, intercalation or strain is crucial for diverse applications. Due to their thinness and mechanical flexibility, 2D materials are increasingly explored for strain engineering, unlocking potential uses in sensors, electrodes, coatings, optoelectronics, spintronics, and straintronics.

With that in mind, we demonstrate two methods to induce and control strain in monolayer $MoS_2$: (i) *substrate interaction modification via native atom intercalation (self-intercalation)* and (ii) *growth on pre-patterned substrates.* We epitaxially grow $MoS_2$ monolayer islands on graphene on Ir(111) using molecular beam epitaxy (MBE) and intercalate it with either S or Mo between graphene and Ir(111). Our Scanning tunneling microscopy (STM) data revealed that S intercalation weakens the $MoS_2$/graphene interaction, while Mo intercalation strengthens it, resulting in distinct island morphologies as well as changes in strain present in $MoS_2$. Utilizing Scanning tunneling spectroscopy (STS) we showed significant shifts in electronic states, exceeding simple rigid band shift. Our numerical calculations linked these shifts to substrate screening, intralayer strain, and $MoS_2$ binding energy per unit cell, correlating well with experimental results.[1] To achieve out of plane bending we synthesized $MoS_2$ on patterned substrates, specifically single-layer graphene on stepped Ir(332), which forms quasi-periodic terraces and step bunches. Monolayer $MoS_2$ islands continuously traverses such structures, conforming to this morphology, thus introducing bending strain which we see in STM. Kelvin probe force microscopy (KPFM), nano Fourier transform infrared spectroscopy (nano-FTIR), and Raman spectroscopy confirmed the presence of strain within this system and revealed significant changes in work function induced by $MoS_2$ islands.

Our findings highlight two pathways to modify strain present in the 2D systems: Self-intercalation, an elegant, non-invasive method to modify strain and enabling bandgap tuning in 2D semiconductors; and a pattern substrate synthesis, a successful bottom-up approach to strain engineering offering promising opportunities for nanoscale device applications.

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# Safe and sustainable-by-design approaches to epitaxial PV cells

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Keywords: LCA, Ecological Risk Assessment, Multijunction cells, III-V, SSbD

Multijunction III-V solar cells have for many years been proposed as a promising PV technology development avenue to increase the efficiency of PV systems in different and novel applications. By incorporating micron-thick layers of III-V materials (gallium, indium, arsenide, phosphide) grown via metalorganic vapor phase epitaxy, these modified cell designs can harvest a broader spectrum of sunlight than conventional silicon PV cells. The benefits of these material innovations in PV design must, however, be carefully balanced with the potential environmental trade-offs of using more complex material structures and energy intensive manufacturing processes to ensure the benefits are not outweighed when all relevant criteria are considered.

We illustrate the use of Life Cycle Assessment (LCA) and Ecological Risk Assessment (ERA) to first evaluate these criteria, and complement the analyses with state-of-the-art techniques in scenario analysis, uncertainty analysis, global sensitivity analysis and multi-objective optimization as decision support tools. The goal of applying such an integrated framework is to improve the safety and sustainability of multijunction III-V/silicon devices from the design stage, while considering all product life cycle stages. In presenting our approach, we place special focus on the necessary complementary application of ERA next to LCA, and on the numerous uncertainties introduced by both types of models. Despite the implementation of large and complex models to assess the environmental impacts and risks and the numerous uncertainties introduced, we demonstrate it is possible to apply a robust framework to simplify the decision making process based only on the most relevant factors, as determined by a global sensitivity analysis.

An additional challenge of making design decisions based on such holistic LCA/ERA models is the numerous indicators that are produced reflecting different environmental criteria which should also be balanced with other criteria such as cost and criticality. With the same data and models, an additional step can be taken to simplify the decision process using multi-objective optimization techniques which substantially reduce the decision space to a smaller subset of optimal solutions. Our work can provide valuable support to technology developers facing similar design choices during low TRL stages, while design changes are still relatively inexpensive to make.

# Considerations on the rebound effects and the technological promise

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Keywords: rebound effects, ICT, environmental impact

The various forms of rebound effects have been unveiled and studied in many sectors of the economy since the seminal papers by Khazzoom [1] and Brookes [2]. The rebound effects are particularly important in the Information and Communication Technology (ICT) sector (see for instance the review of literature by Gossart [3]) for which the greenhouse gas emissions keep increasing despite huge energy efficiency gains for components and systems [4].
In this talk, I will introduce the concept of rebound effects and focus on the peculiarities of the ICT sector in this respect. The environmental impact of a technology depending obviously on the various use cases and their deployments, I shall question the validity of an hypothetical intrinsic environmental virtue attached to a technological innovation. As a conclusion and perspective, I will share some considerations on what I think this implies for the way we researchers discuss the potential economic, social and environmental impacts of the innovations we develop in the lab.

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# Strategies for Improvement of GaAsBi Quantum Well-Based Laser Performance for Emission above 1000 nm

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Keywords: MBE, laser diode, quantum well, GaAsBi, near-infrared

Near-infrared (NIR) is a frequently exploited wavelength area due to its wide range of applications. Spectral lines in the 800 to 1100 nm region are of particular importance due to their applications in sensing. One possible example is matching the optical path lengths of emitted light by using an 1100 nm laser in combination with 800 nm to decrease the inaccuracies of pulse oximeters [1]. While the 800 nm emission is easily achieved with AlGaAs-based semiconductor emitters, the longer wavelengths are more challenging.

The current solutions for emission above 1000 nm are mainly based on the InGaAs emitters grown on the GaAs platform. The issue arises with tuning the emission of this material to longer wavelengths, where high In content has to be introduced, resulting in lattice mismatch dislocations. A possible candidate for emission in the region around 1000 nm can be GaAsBi grown on GaAs substrate. This alloy has a plethora of advantageous properties. The rapid bandgap reduction of up to 88 meV/%Bi allows small Bi contents to be used for covering longer wavelengths. In this way, a dislocation-free crystalline structure can be achieved [2]. At the same time, the possible suppression of Auger losses at Bi contents larger than 11 %, low-temperature sensitivity of emission wavelength and room temperature operation could greatly increase the efficiency of laser systems in the NIR [3, 4]. Despite that, the success of GaAsBi-based emitters is held back by its complicated growth conducted at low temperature (<440 °C Bi incorporation threshold) and a stoichiometric As/Ga [5]. The consequence of such growth is an abundance of point defects resulting in low laser power and high threshold current. This work focuses on strategies for improving the laser parameters and was carried out in two main avenues: (i) optimizing the design of the grown quantum structure and (ii) improving device processing protocol. First, the reduction of the total defectiveness of the gain area was achieved by designing thinner GaAsBi QWs with larger Bi content (>7%), which facilitated the reproducibility of high emission intensity. Additionally, our findings on parabolically graded spacers used for significant increase of PL by enhancing the carrier trapping efficiency was implemented [6]. Finally, substrate thinning procedure was employed to reduce the losses caused by the defects in the doped GaAs substrates and worse heat dissipation. Combination of all these techniques allowed us to decrease the threshold current by more than 30 times in magnitude and achieve a peak output power of over 140 mW under pulsed electrical excitation (50ns at 1kHz) for FP-type laser diodes operating above 1000 nm.

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# Optimized MSM Photodetector Design: The Influence of Barrier and Digital Graded Superlattice Layers

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Keywords: InGaAs, MSM photodetector, barrier layer, digital graded superlattice layer

$In_xGa_{1-x}As$ (x=0.53) based metal-semiconductor-metal (MSM) photodetectors have several advantages such as ease of fabrication, ease of integration, and low capacitance per unit active area. Different MSM photodetector structures, such as with barrier and digitally graded superlattice layer, are critical in determining device performance [1,2].

This study aims to fabricate MSM photodetector structures with an $In_yAl_{1-y}As$ (y=0.52) barrier layer and a digitally graded superlattice (DGSL) layer with an $In_yAl_{1-y}As/In_xGa_{1-x}As$ (x=0.53, y=0.52) 9:1 thickness ratio. In the initial phase of the study, the layers in the photodetector structure were simulated in 3D using Silvaco TCAD, and the optimum layer thicknesses were determined. A review of the literature shows that the digitally graded superlattice layer of the MSM photodetector structure was extremely thin, which is why it has traditionally been grown using the MBE system. However, this study demonstrated that the DGSL layer can also be grown using the MOVPE system while maintaining high crystal quality, even with a thickness variation of 1 nm.

In addition, to investigate the effect of the barrier layer and the digitally graded layer on device physics, MSM-1 structures containing only the absorption layer, MSM-2 structures containing the barrier layer, and MSM-3 structures containing the absorption, barrier, and digitally graded superlattice layers were grown and fabricated (Figure 1). In this study, the effect of the MSM photodetector layer structure on device performance was also investigated.

This study aims to investigate the compatibility of simulations and experimental studies, with a focus on photodetector simulations, to enhance and support future experimental research.

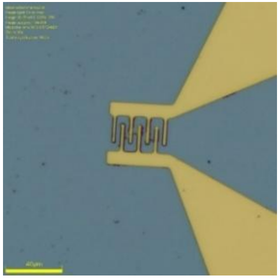

**Figure 1.** Optical images of the MSM photodetector

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# Fabrication and Characterization of Iron Titanate Thin Films as a Potential Tunnel Barrier for Magnetic Tunnel Junction (MTJ's)

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Keywords: Thin films, spintronics, magnetism

Spintronics addresses rising power dissipation in electronic circuits by offering advantages such as 0% standby leakage, low power consumption, unlimited durability, non-volatility, and compatibility with CMOS technology [1]. In this research work focuses on magnetic tunnel junctions (MTJs) in spintronics, investigating the barrier layer for efficient electron spin transfer, crucial for Magnetic Random Access Memory (MRAM). Iron titanate thin films have attracted research interest due to their potential applications in spintronic devices [2]. An applicationoriented electrodeposition technique was used to prepare iron titanate thin films with varying electrolyte molarities [1,2]. XRD results reveals the amorphous behavior of As-deposited thin films. Magnetic field (MF) annealing improved the structural and magnetic properties, the Fe2TiO4 phase was observed, confirming a spinel structure with increased crystallite size and strengthened phase as molarity increased. Magnetic analysis using a vibrating sample magnetometer (VSM) showed soft ferromagnetic behavior in annealed thin films, while the as deposited thin films show para-ferromagnetic mixed behavior. As-deposited films had lower saturation magnetization compared to annealed films.

In conclusion, $Fe_2TiO_4$ thin films fabricated via electrodeposition demonstrate significant potential for future spintronic devices specifically in the advancements of MRAM technology.

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# Epitaxial Growth of LSMO Thin Films by Solid State Pulsed Laser Deposition for MEMS Applications

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Keywords: Pulsed Laser Deposition, Magnetic Thin Films, X-ray Diffraction, MEMS

Solid state lasers (SSL) present some advantages, for example in terms of use and maintenance costs, over excimer lasers that are widely employed in pulsed laser deposition (PLD) of complex oxides. However, the quality of the films is generally lower, limiting their use in materials research. Yet, the use of solid state lasers might be suitable for the realization of microelectromechanical systems (MEMS) based on complex oxides. We report the growth of $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) thin films by PLD with SSL. LSMO is a magnetic compound with potential applications in the development of MEMS sensors with resonating magnetic elements.

LSMO films are deposited on $SrTiO_3$ substrates using a Nd:YAG laser and non-linear optics to generate a 266 nm wavelength laser beam of up to 35 mJ/pulse and focused on a LSMO sintered target. We perform *in-situ* characterization of the film growth by reflection high energy electron diffraction and analyse the surface morphology by atomic force microscopy. The presence of particles at the surface of the sample is critical for the realization of thin film devices and multilayers and it depends on the laser fluence. Built-in stress of the films is another key factor when developing resonating mechanical structures, as it affects both the mechanical eigenfrequencies and the quality factors of the resonators [1,2,3]. Structural quality, film lattice parameters and built-in stress are analysed by X-ray diffraction and mechanical measurements on suspended LSMO microbridges.

Our preliminary results show that PLD with SSL is well-suited for the realization of micromechanical devices with single LSMO films with prospects for integration with other oxide layers.

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# Electrodeposited Zirconium Titanate Thin Films: Structural, Magnetic, and Dielectric Properties for Spintronic Applications

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Keywords: Thin films, spintronics, magnetism

Zirconium titanate (ZrTiO4) thin films have emerged as a cornerstone material in the advancement of spintronic devices, owing to their exceptional structural, magnetic, and dielectric properties [1,2]. This study harnesses a precise electrodeposition technique to fabricate ZrTiO4 thin films, meticulously varying the molarity of electrolytes from 0.01M to 0.05M. X-ray diffraction (XRD) analysis reveals a transition from amorphous behavior at 0.01M to the formation of phase-pure, orthorhombic ZrTiO4 at higher molarities, with a notable increase in crystallite size, indicative of enhanced phase stability. Vibrating Sample Magnetometer (VSM) measurements demonstrate a pronounced soft ferromagnetic behavior, with an impressive saturation magnetization peaking at 29 emu/cm$^3$ at 0.05M. Dielectric studies reveal a significant dielectric constant of 180 at log f=2 and a minimal tangent loss of 0.02 at 0.05M, showcasing superior dielectric performance. Cole-Cole plots further elucidate the dielectric properties, indicating dominant grain boundary resistance. The comprehensive analysis underscores the potential of ZrTiO4 thin films as pivotal components in nextgeneration spintronic devices, offering unparalleled structural integrity, magnetic prowess, and dielectric efficiency [2].

These findings pave the way for the integration of ZrTiO4 thin films in high-performance, energy-efficient spintronic applications, marking a significant leap forward in material science and device engineering.

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# Ge-on-Si bias-tunable dual-band photodetector for solvents recognition

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Keywords: Infrared sensing, Ge-on-Si, dual-band photodetector, solvent discrimination, multi-band imaging

Light sensing beyond the visible spectra has always played an important role in scientific advances. Connecting two photodiodes made of different semiconductors in a back-to-back configuration creating a dual-band detector, allows the acquisition of information in two different spectral bands depending on the semiconductor bandgap and external voltage bias.

Dual-band photodiodes based on Group IV materials such as silicon (Si) and germanium (Ge) can cover the visible (VIS) and near infrared (NIR) ranges (λ = 400 - 1100 nm) and short-wave infrared (SWIR) ranges (λ = 800 - 1600 nm), respectively, allowing independent data collection from the SWIR/VIS-NIR ranges (see Figure 1 a, b). Thus, data acquired from visible (VIS) and infrared (IR) ranges can be combined to retrieve information that neither band can provide by itself.

The device responsivity can then be tuned by the magnitude and polarity of the voltage bias, achieving an open-circuit voltage ($V_{0C}$) when the produced photocurrent vanishes, $I_{ph} = 0$. This open-circuit voltage depends on the thermal voltage, $V_T$, and the natural logarithm of the ratio between the photo and dark currents of the individual photodetectors.

$$V_{0C} = V_T \ln\left(\frac{I_{ph}^{Ge}}{I_{ph}^{Si}}\frac{I_0^{Si}}{I_0^{Ge}}\right)$$

The $V_{0C}$ values are dominated by variations of the $I_p{}^{Ge}{}_h / I_p{}^{Si}{}_h$ ratio, and such feature can be exploited to discriminate between solvents perfectly transparent in VIS but with distinct absorption in IR, enabling the recognition of different solutions with a resolution of a few mV on $V_{OC}$, as shown in Figure 1c. Furthermore, the simple device structure and the Si-Ge compatibility allow for compact, reliable, scalable, and reproducible detectors that can be produced at low cost and operate at low voltage bias. In summary, we demonstrate a compact and scalable Ge-on-Si dual-band detector capable of discriminating between different solvents without mechanical or dispersive element thus reducing the necessity of complex optical assemblies to cover broad light spectra or the need for different detectors.

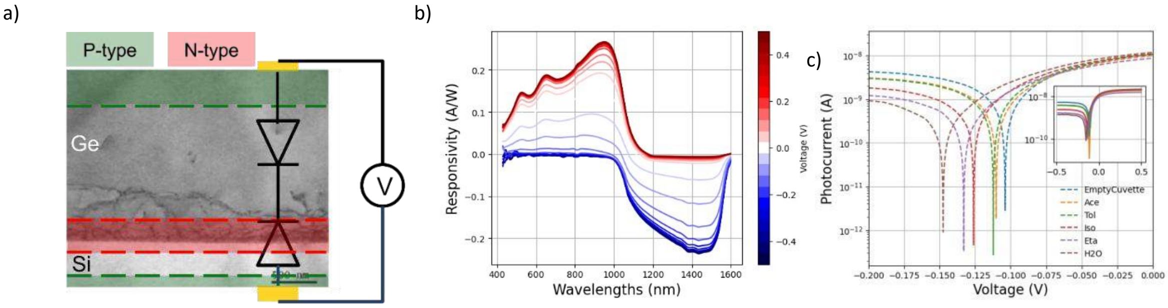

Figure 1- (a) Schematic representation of the dual-band detector (b) Device responsivity measured for several voltage bias (c) measured photocurrent-voltage curves for the different solvents.

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# Advanced Functional $Cd_xZn_{1-x}S$ Nanocomposites: Comparative Study of Sonochemical and SILAR Synthesis for Application-Oriented Materials

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Keywords: $Cd_xZn_{1-x}S$ nanostructures, band gap value, optical properties, structural properties

Composite elements from II–VI groups have a wide range of possible uses in optoelectronics and optics. With band gap values of 2.42 eV and 3.8 eV, respectively, CdS and ZnS stand out among these groups. Among the most researched materials for organic pollution degradation and solar applications are CdS and ZnS binary semiconductor complexes. The primary goal is to compare the physical characteristics of $Cd_xZn_{1-x}S$ nanocompounds made using the SILAR and sonochemical approaches. Using the same stabilizers (PVA) with different composite materials ($Cd_{0.2}Zn_{0.8}S$; $Cd_{0.4}Zn_{0.6}S$; CdS), while using different stabilizers (PVA, 3-MPA, and styrene) for the same combination ($Cd_{0.4}Zn_{0.6}S$) (by sonochemical approach) and different composite materials ($Cd_{0.1}Zn_{0.9}S$; $Cd_{0.2}Zn_{0.8}S$; CdS) that are synthesized at room temperature and at different synthesis temperatures (45°C and 65°C) for $Cd_{0.2}Zn_{0.8}S$/PVA composite materials (by SILAR approach). The effect of technological parameters (synthesis method, temperature, capping agents) on the structure and physical properties of the produced binary and ternary $Cd_xZn_{1-x}S$ nanomaterials may then be investigated.

The primary peaks in the diffraction pattern of the sonochemical method are those of CdxZn1-xS, but faint intensity peaks typical of the stabilizers used are also visible. Furthermore, it was noted that particles with a high degree of crystallinity are generated in the sonochemical technique, resulting in more strong diffraction peaks than in the SILAR approach. This is linked to better crystallization using ultrasonic waves and fewer faulty structures. Ternary compounds, $Cd_xZn_{1-x}S$, were created in the hexagonal phase when both techniques were being used. However, the SILAR strategy produced the hexagonal phase of CdS during the production of the binary compound (at a value of x equal to 1), while the sonochemical approach produced the cubic phase. That is, the synthesis of the hexagonal phase of CdS via the SILAR approach is advantageous from an energy perspective, but the sonochemical approach uses enough energy from the ultrasonic waves to generate the cubic phase in the binary compounds. The sonochemical method produces nanocomposites in the form of small and large crystallites, as can be seen from the SEM images. The SILAR method produces nanocomposites in the form of fragments (layers) and adhesion to the surface, which is connected to the polymer surface.

The SILAR approach (3.05 eV and 3.45 eV) and the sonochemical method (2.80 eV and 2.25 eV) both produced lower $E_g$ values for nanocomposites with the same composition ($Cd_{0.2}Zn_{0.8}S$/PVA and CdS/PVA). The samples obtained using the SILAR approach showed a blue shift, while the samples obtained using the soochemical method showed a red shift. The mechanism of interaction between various forms of electrolyte solution (environment) and nanoparticles is linked to the variation in Eg value based on the production method. Accordingly, these effects are associated with electrical potential changes brought on by interactions with flaws, covers, broken bonds, shape, and other related elements. Composite materials' potential for use is increased by their capacity to change their optical characteristics based on technological circumstances.

# FeGa/MoSe$_2$/hBN and AlO$_x$/FeGa/MoSe$_2$/hBN heterostructres for combination of magnetostriction effects with 2D materials

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Keywords: characterization; magnetostriction effect; 2D materials; photoluminescence

This study investigates the synthesis of FeGa/MoSe$_2$/hBN and AlOx/FeGa/MoSe$_2$/hBN heterostructures. Layers with Al, FeGa, and MoSe$_2$ were grown using Molecular Beam Epitaxy (MBE), while hBN was in form of flakes exfoliated from bulk and deposited on SiO$_2$/Si substrate. After removing structure from ultra high vacuum 3 nm Al layer turned to AlO$_x$. Composition of FeGa was calibrated as Fe$_{0.8}$Ga$_{0.2}$, which is optimal for observation of magnetostriction effects.

The reference films and full heterostructres were analyzed using Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM), low temperature Photoluminescence (PL), Raman Spectroscopy, and magneto-optical spectroscopy to explore their structural, morphological, and optical properties. The results reveal that GaFe layers significantly suppress MoSe$_2$'s photoluminescence due to metal-induced quenching, with a 5 nm GaFe layer drastically reducing PL intensity. At 10–20 nm GaFe thickness, MoSe$_2$'s optical response disappears. Al$_2$O$_3$ improves interfacial stability, enhancing surface homogeneity. AFM analysis reveals MoSe$_2$'s irregular layering on hBN, influencing its optical behavior. These findings demonstrate the crucial impact of GaFe thickness on MoSe$_2$'s magneto-optical properties, offering insights for spintronic and optoelectronic device design.

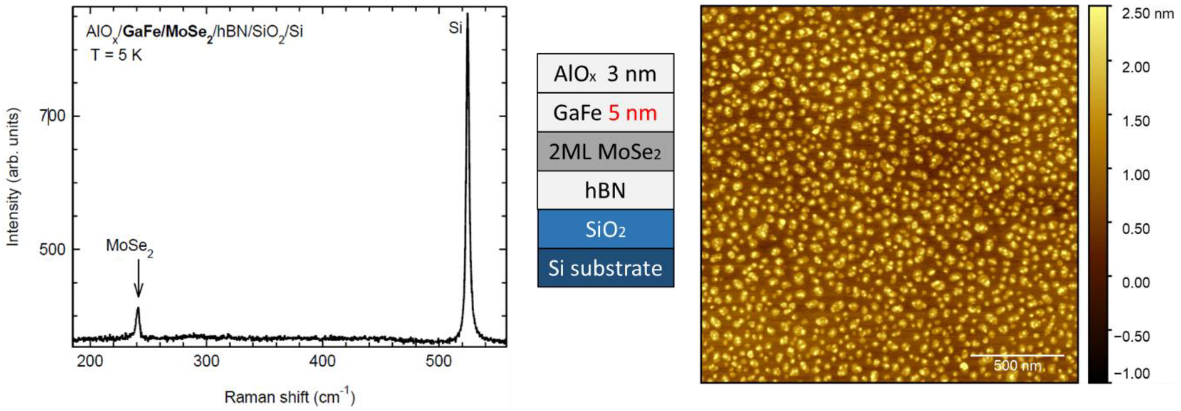

**Figure 1.** Raman scattering spectrum and AFM image of AlO$_x$/GaFe/GaFe/MoSe$_2$/hBN/SiO$_2$/Si heterostructure.

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# FDTD simulations of $In_xAs_{1-x}P$ quantum dots in zinc-blende InP nanowires for efficient telecom band emission

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Keywords: quantum dots in zinc-blende nanowires, InP-based material system, vapour-liquid-solid chemical beam epitaxy, optical properties, numerical simulations

Quantum dots (QDs) are known as excellent single photon emitters. Recently, it was shown that $In_xAs_{1-x}P$ QD in a zinc-blende InP nanowire (NW), grown by Chemical Beam Epitaxy technique, can emit at telecom wavelengths [1]. A properly tailored NW embedding a QD acts as a single mode waveguide, causing high extraction efficiency (EE) upwards by enhanced directionality of QD spontaneous emission [2]. The above mentioned properties are beneficial for efficient light coupling to an optical fiber and realization of quantum communication protocols over large distances.

The aim of this study is to optimize the geometry of this QD-NW system within the parameters range limited by the growth technology to achieve maximal EE within numerical aperture (NA) of 0.4 and 0.65 used in the experiment. Here, we present numerical calculations using the finite-difference time-domain (FDTD) method in commercial Ansys Lumerical software [3]. The QD was modelled as an electric dipole placed on NW axis and polarized perpendicularly to it. The NA of detection optics was implemented by analyzing the angular dependency of a far-field emission pattern. The optimized geometry parameters were: NW length, InP shell thickness, taper angle and QD position along the NW axis. It was concluded that the optimal geometry consist of 3 segments: a bottom untapered part with the QD placed in the anti-node of the waveguide mode, a tapered middle part for efficient light outcoupling and a tip with a gold droplet on top, being a consequence of the growth process. The influence on the EE of a bottom gold mirror and distributed Bragg reflectors made in different material systems compatible with InP were simulated. It was shown that both solutions can be implemented to increase the EE by a factor of 2. For fully optimized NW geometry and a bottom gold mirror a theoretical EE value of 46% with Purcell factor 1.46 for 0.65 NA was obtained at 1.5 µm. In order to verify the simulations with experimental data, micro-photoluminescence spectra were collected from samples with the same QDs but different NW shell thicknesses. The integral intensity of emission turned out to be the highest for NWs with shell thickness closest to the one calculated as optimal.

We acknowledge financial support from the European Innovation Council (EIC) Pathfinder under Horizon Europe. Grant number: 101185617.

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# Ranges and limits of p-doping in Y:$HfO_2$ – an electronic structure study by HAXPES

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Keywords: HAXPES, oxygen vacancies (OVs), Hafnia, p-doping, ferroelectric

Ferroelectric $HfO_2$-based thin films exhibit huge potential for the next generation of nonvolatile memory applications, such as FeRAM or Fe-FET. However, the application of $HfO_2$-based thin films as active ferroelectrics (FE) in devices still faces reliability issues like wake-up, imprint, and fatigue. The concentration of oxygen vacancies (OVs) plays a dual role: it stabilizes the FE phase while also contributing to breakdown during electrical cycling.

For p-doped $HfO_2$, the electronic constraints governing OV formation remain an open experimental question. In this study, we investigate Y-doped $HfO_2$ (Y:$HfO_2$) thin films synthesized via atomic layer deposition (ALD), with Y concentrations ranging from 2.9% to 17.1%.

Using hard X-ray photoelectron spectroscopy (HAXPES), we analyze the local chemistry and global electronic properties of Y:$HfO_2$, focusing on the Hf 4f core level. The presence of $Hf^{3+}$ components and rigid binding energy (BE) shifts serve as key indicators of OV formation. Our findings reveal an OV formation trend as a function of Y doping. Notably, above a critical doping threshold, Y (p-dopant) incorporation no longer exhibits a p-doping effect due to the excessive formation of OVs, fundamentally altering the electronic properties of the Y:$HfO_2$ layer.

# Second-order Phase Transition and Magnetic Anisotropy-Driven Magnetocaloric and Giant Magnetoresistance Effects in La-Ba-Mn-Ti-O Epitaxial Thin Films

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Keywords: Giant Magnetoresistance, Epitaxial thin film of manganite,

Epitaxial La-Ba-Mn-Ti-O (LBTMO) thin films, approximately 95 nm in thickness, were deposited onto SrTiO3 (STO) (001) substrates using a pulsed laser deposition technique. High-resolution X-ray diffraction (HRXRD) and transmission electron microscopy (TEM) studies revealed that the films exhibit a four-fold symmetry around the [001] direction. Doping with a small amount of titanium and the induced stress due to lattice mismatch between the thin film and the substrate both contribute to a reduction in the Curie temperature ($T_C$), as compared to the pristine compound, and consequently lower the temperature at which the maximum magnetoresistance effect (MRE) occurs. We have developed a thin film structure exhibiting a maximum MRE at room temperature, which is a key requirement for many practical applications. The easy axis of magnetization lies within the film plane, along the [100] direction of the (001) substrate. The magnetic entropy change ($\Delta_{SM}$), associated with the second-order magnetic phase transition, was determined through magnetization measurements conducted in the temperature range of 210–350 K under varying magnetic fields. The relative cooling power (RCP) of this film is approximately 220 J kg$^{-1}$, slightly lower than that of bulk Gd (410 J kg$^{-1}$) for a 50 kOe field change, making the LBTMO ferromagnetic thin films a promising candidate for micro/nanomagnetic refrigeration around room temperature.

# Growth optimization of $Sb_2Se_3$ thin films on ZnSe/ITO substrates

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Keywords: close space sublimation method, $Sb_2Se_3$ thin films, SEM, EDS, XRD

The epitaxial growth of antimony selenide ($Sb_2Se_3$) thin films by close space sublimation (CSS) method on the ZnSe/ITO substrates has been reported. The morphological, composition and structural properties of the films were studied as a function of the substrate temperature. Experimental data indicate that $Sb_2Se_3$ films have Sb-rich composition and polycrystalline structure. The surface morphology is affected by the substrate temperature and the increase of temperature converts to larger $Sb_2Se_3$ grains (Figure 1). The source temperature was kept at 550℃. Commonly, the morphology comprised 1D/2D grains as a result of low structural dimensionality of $Sb_2Se_3$.

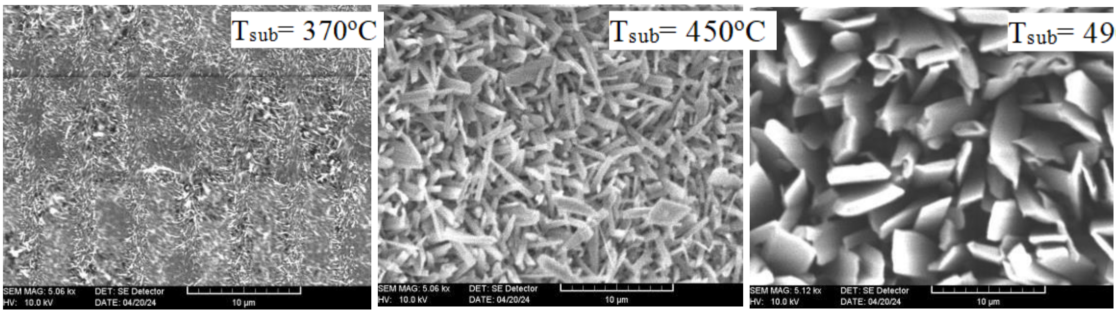
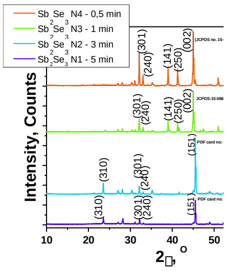


**Figure 1** SEM images of $Sb_2Se_3$ in function of substrate temperature.

X-ray diffraction (XRD) patterns were recorded using a Bruker d8 advance diffractometer with $CuK_\alpha$ radiation ($\lambda$ = 1.5406 Å, 40 kV, 40 mA), for a set of samples obtained at $T_s$=450°C and $T_{ev}$=550°C, varying time of the deposition. The orientation parameter of a crystalline plane (hkl) was quantitati- vely described by the texture coefficient ($TC_{hkl}$). The orientation of the films was found to be vertical (*hkl*, *l*≠0) when c-axis is inclined to the substrate and $R_O=\sum I_{hk0}/\sum I_{hkl}=0$.

**Table 1** Microstructural parameters of $Sb_2Se_3$ thin films



| Samples $T_s$=450°C $T_{ev}$=550°C | Time of deposit, sec. | d(Å) | D, (nm) | Strain (%) $10^{-3}$ | Peak intensity |
|---|---|---|---|---|---|
| $Sb_2Se_3$_N1 | 30 | 1.9923 | 120.5 | 4.45 | 2368 |
| $Sb_2Se_3$_N2 | 60 | 1.9911 | 78.5 | 6.83 | 5728 |
| $Sb_2Se_3$_N3 | 180 | 4.0241 | 48.2 | 11.2 | 4111 |
| $Sb_2Se_3$_N4 | 300 | 4.0241 | 34.1 | 15.9 | 5458 |

**Figure 2** XRD analysis of $Sb_2Se_3$ thin films

XRD analysis suggests that grain orientation can be altered by changing the time of deposition not only by modification the deposition conditions.

# Low-temperature growth of Al monolayer on 7×7 reconstructed Si (111) surface by molecular beam epitaxy

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Keywords: Epitaxy growth, (7x7) reconstruction, monolayer, nucleation layer, Aluminum

AlN serves as a nucleation layer for the growth of III-nitride materials on Si (111). The quality of these heterostructures is critically influenced by the initial film growth conditions, particularly the extent and morphology of Si surface coverage by Al. In this study, low-temperature molecular beam epitaxy (MBE) was employed to achieve uniform coverage of the (7×7) reconstructed Si (111) surface with Al. Surface structure evolution during Al deposition was monitored using reflection high-energy electron diffraction (RHEED). The low-temperature MBE process saturates Si dangling bonds with a single layer of Al atoms while preserving the original (7×7) reconstruction. X-ray photoelectron spectroscopy (XPS) confirmed the complete saturation of Si dangling bonds by Al adatoms. Atomic force microscopy (AFM) was used to characterise the roughness of air-exposed samples and evaluate the density of undesired Al nanoclusters. These films will serve as a platform for subsequent layer-by-layer MBE deposition of AlN at low temperatures, followed by metal-organic chemical vapour deposition (MOCVD) to grow thicker films.)

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Pisa, May 2025

# Fabrication of blue phosphorene

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**Keywords:** phosphorus deposition, 2D materials, GaP, blue phosphorene, LEEM, LEED

Phosphorene, a 2D material derived from black phosphorus, has attracted significant interest due to its unique electronic and optical properties, making it a strong candidate for applications in nanoelectronics, optoelectronics, and energy storage [1]. Despite its potential, the controlled synthesis of phosphorene remains challenging due to its strong interaction with metallic substrates [2]. Understanding the growth mechanisms is crucial for optimizing phosphorene fabrication.

In this study [3], we combine in situ Low-Energy Electron Microscopy (LEEM), Low-Energy Electron Diffraction (LEED), Scanning Tunneling Microscopy (STM), and X-ray Photoelectron Spectroscopy (XPS) to investigate the deposition and structural evolution of phosphorus on a Cu (111) substrate. Our results reveal that during the initial stages of phosphorus deposition, phosphorus atoms interact strongly with the copper surface, leading to the formation of copper phosphide rather than direct phosphorene growth. LEEM imaging and LEED patterns confirm the presence of this intermediate structure. As phosphorus deposition continues, we observe a structural phase transition, ultimately leading to the emergence of phosphorene. The influence of the used deposition method plays key role on the result. We generate flux of phosphorus dimers ($P_2$) by the thermal decomposition of gallium phosphide (GaP). The use of $P_2$ molecules [3], rather than $P_4$ molecules [4], plays a crucial role in formation of phosphorene and in facilitation of the phosphide>phosphorene transformation.

These insights provide a deeper understanding of the fundamental mechanisms of phosphorene growth on metallic substrates and offer guidelines for the scalable synthesis of phosphorene.

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# Single-phase κ-$Ga_2O_3$ films deposited by Metal-Organic Vapor Phase Epitaxy on GaAs and ternary $B_xGa_{(1-x)}As$ templates

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Keywords: κ-$Ga_2O_3$; Polymorphism ; Heterostructure; MOVPE; III-V semiconductors; BGaAs

κ-$Ga_2O_3$ epitaxial layers were grown on (001) p-type GaAs and $B_xGa_{(1-x)}As$ /GaAs templates using metal-organic vapor phase epitaxy (MOVPE). The films were analyzed by X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Columnar growth of orthorhombic κ- phase grains was observed on the GaAs substrate and on the $B_xGa_{(1-x)}As$ /GaAs template, coalescing into a closed film. For the first time, a single pure-phase κ-$Ga_2O_3$ film was deposited on such substrates. The boron (B) in the ternary alloy tends to accumulate at the upper surface of the template, due to segregation, which leads to B diffusion into gallium oxide and formation of a thin amorphous oxide (*a*-BGaO) interlayer between $Ga_2O_3$ and the template.

The new type of heterojunction will enable the development of new active layers for photodetectors and solar cells in the UV, visible and infrared regions.

# Energy storage and harvesting performance of Aurivillius oxide thin films grown by pulsed laser deposition

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Keywords: Relaxor, Aurivllius, Energy storage, Photovoltaic

Aurivillius ferroelectrics, a class of layered perovskite-like materials, exhibit excellent fatigue resistance and a high breakdown electric field, making them promising candidates for dielectric energy storage. However, their layered architecture poses significant challenges in growing single-crystalline thin films, limiting their integration into oxide-electronic devices. Additionally, achieving high energy storage performance at medium and low electric fields remains difficult due to polarization suppression caused by polar nanoregions in relaxors.

This study investigates five-layered, lead-free (SrB4La)(Ti4Fe)O18 (SBLFT) relaxor ferroelectric films, demonstrating enhanced polarization and breakdown strength. Strain engineering through controlled thickness variation (60–320 nm) optimizes inter-layer distortions and interactions, significantly improving relaxor behavior and breakdown strength. As a result, the films achieve an ultrahigh recoverable energy storage density of 98 J/cm$^3$, 80% efficiency, and a breakdown field of 3100 kV/cm, with excellent thermal (-20 to 120°C) and cycling ($10^8$ cycles) stability. Finite element simulations further validate performance.

Additionally, ITO/SBLFT devices exhibit a switchable photoresponse with a high ON/OFF photocurrent ratio, an open-circuit voltage of 0.15 V, and a rapid zero-bias photoresponse reaching ~3 µA. The study presents detailed insights into the system's energy storage and photovoltaic performance.

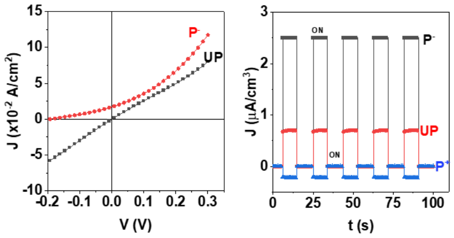

Illustration of photovoltaic characteristics of ITO/SBLFT/Platinized Si.

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# Impact of Bismuth Dopant Layers on the Optical Behavior of GaAs/AlAs Quantum Wells

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Keywords: bismuth, δ-doping, GaAs/AlAs, quantum wells, photoluminescence, photoreflectance

As semiconductor devices become smaller and more efficient, advanced growth techniques are essential for optimizing their properties. Among these, δ-doping offers precise control over the optical and electronic characteristics of materials by confining dopant atoms to a few atomic monolayers (ML). While δ-doping of GaAs/AlAs quantum wells (QWs) with beryllium has been extensively studied [1], the impact of bismuth (Bi) deposition in ML remains unexplored.

This study investigates the optical properties of 5 nm-thick GaAs/AlAs QWs with 1, 4, 6, and 8 ML of Bi using temperature-dependent photoluminescence (PL) and photoreflectance (PR) spectroscopy. Low-temperature PL measurements reveal new energy states below the QW bandgap (Fig. 1a). PR spectra (Fig. 1b) show that up to 4 ML of Bi induces a bandgap blueshift and enhances thermal stability, whereas depositing 6 ML or more leads to the formation of a narrow (<5 nm) GaAsBi/GaAs QW within the existing structure. These results offer valuable insights into how bismuth atomic layer deposition modifies the optical characteristics of quantum wells and highlights the need for further research.

This work was supported by the Research Council of Lithuania (LMTLT), agreement No. S-LT-TW-24-8.

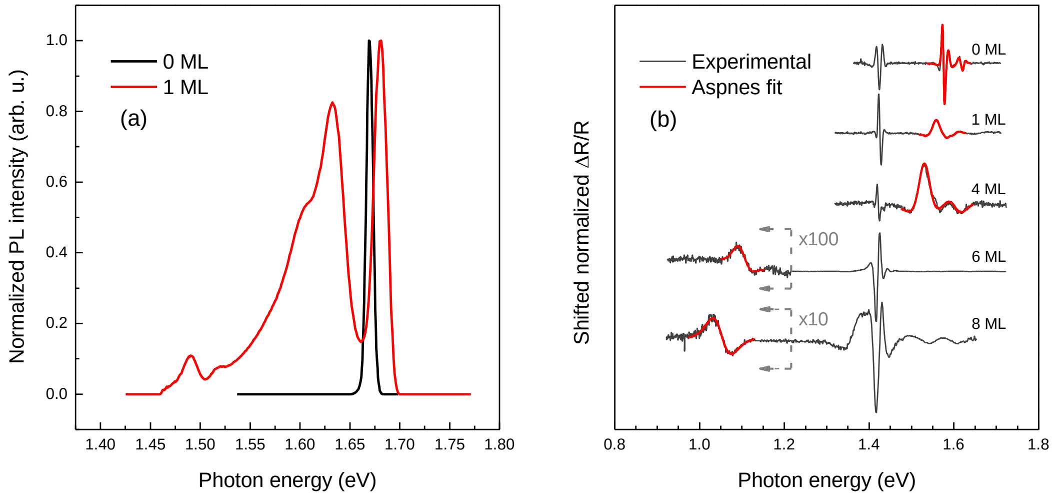

**Figure 1.** (a) Low-temperature PL spectra of 25 x 5 nm-thick GaAs/AlAs QW structures with 0 and 1 ML of Bi. (b) Room-temperature PR spectra of GaAs/AlAs QW structures containing 0, 1, 4, 6, and 8 ML of Bi, fitted to Aspnes' function [2].

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# Growth and transfer approaches to back-gated oxide heterostructure devices

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Keywords: 2DEG, Back-gating, freestanding film, remote epitaxy

Complex oxide heterostructures with multiple functionalities are extensively explored by researchers to build the next-generation electronic devices. Among them a prominent candidate is $LaAlO_3$(LAO)/$SrTiO_3$(STO) system. It offers interfacial 2-dimensional electron gas (2DEG) which is conducting, superconducting and shows magnetism [Nature 427, (2004)]. Significant research efforts are being put to modulate the conductivity of 2DEG and to explore the different phases in this system, however tuning the 2DEG in standard LAO/STO interfaces requires gate voltage exceeding up-to few hundred volts [Science 313, (2006)], which makes the device challenging for the practical application. To address this issue alternative approaches are being explored based on the development of all-thinfilm devices, freestanding oxides, and remote epitaxy using graphene as interlayer [1].

In this study, we present different approaches to arrive at back-gate-type LAO/STO heterostructures with the goal to reduce the required gate-voltages. In the first approach we attempted to deposit $LaAlO_3$/$SrTiO_3$ bilayer onto a graphene-coated $SrTiO_3$ (STO) substrates, where the graphene layer could serve as a back-gate. We successfully observed the layer-by-layer growth of LAO on graphene buffered STO but detecting and preserving the graphene underneath these bilayers is still very challenging due to delicate nature of graphene in presence of oxygen. Our second approach is based on the transfer and $TiO_2$ termination of free-standing STO lamella[2]. We successfully grew LAO on these lamellas at very low background pressure and observed high electron density based on the redox response of the transferred STO lamella. By transferring such freestanding singly terminated STO lamella on a conducting substrate like silicon (Si) and growing LAO at higher pressure, it may be possible to induce the desired electronic charge-transfer 2DEG, where Si can function as a back-gate allowing electric field control of the 2DEG. In this poster contribution, we will discuss the benefits and occurring challenges in the sample synthesis and processing of such devices.

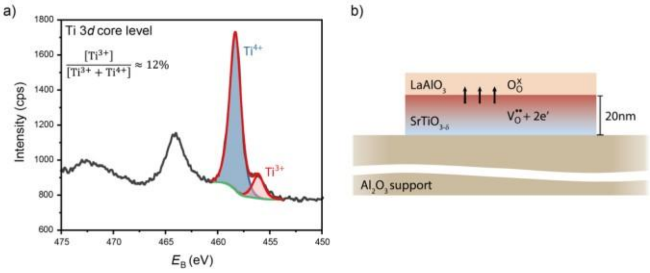

*Figure 1 a) XPS spectra to observe 3d core level for 5UC LAO grown on singly $TiO_2$ terminated 20nm STO layer transfered on saphire. b) Schematic diagram of electron generation in the bulk of 20nm STO lammella (Wohlgemuth, Nayak, et al., submitted, ,preprint available under this link 10.26434/chemrxiv-2025-rcrq6 )*

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# Mechanisms of Temperature-Dependent CO Adsorption on $BaTiO_3$(001): Surface Stability and Gas Sequestration Potential

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Keywords: carbon monoxide, ferroelectric surfaces, barium titanate, adsorption-desorption, X-ray photoelectron spectroscopy, low energy electron diffraction

Using photoelectron spectroscopy, this work examines the reversible adsorption and desorption of carbon monoxide (CO) on BaO-terminated $BaTiO_3$(001) surfaces. The non-dissociated form of CO is adsorbed, and the adsorption geometry changes with temperature. CO adsorbs on top of surface barium atoms below room temperature, on top of surface oxygen above normal temperature, and on top of three oxygen atoms at high temperatures to produce a "hollow" site adsorption. At lower temperatures, the adsorption rate rises by 30%, with around one CO molecule adsorbed for every ten surface unit cells. When the substrate is heated above the Curie temperature, CO is totally desorbed, demonstrating the critical function of ferroelectric polarization in the adsorption process. Repeated cycles of CO adsorption and desorption do not cause the $BaTiO_3$(001) surface to become unstable, indicating that it may find use in controlled CO removal. According to the study, an increase in surface band bending indicates that the interaction of CO with $BaTiO_3$ promotes surface polarization. Further exploration of the adsorption mechanisms and its uses for CO sequestration and other gases is encouraged through theoretical studies.

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# Direct growth and application of 2D single crystals of MXenes

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Keywords: Chemical vapor deposition, Molecular beam epitaxy, $Mo_2C$, SEM-EDS, Nano-SAM (scanning Auger Microscopy).

This work represents a comprehensive exploration of $Mo_2C$ MXene synthesis. We employed an advanced setup, specifically Ultra-High Vacuum Chemical Vapor Deposition (UHV-CVD) and Ultra-High Vacuum Scanning Electron Microscopy (UHV-SEM), for the direct growth of two-dimensional (2D) single crystal MXenes. Our primary objective was to gain insight into the surface properties of $Mo_2C$. We utilized analytical techniques such as Scanning Electron Microscopy (SEM), and Energy-Dispersive X-ray Spectroscopy (EDS), Nano-SAM (scanning Auger Microscopy). Our observations revealed that, at elevated temperatures, copper (Cu) droplets coexisted with needle-like molybdenum (Mo) structures. However, a detailed understanding of such dynamics is still missing.

Therefore, the integration of Molecular Beam Epitaxy (MBE) apparatus with a Mo electron beam cell, direct epitaxial growth of $Mo_2C$ MXenes can be studied. Incorporating the vertical UHV e-beam evaporator enhances the method performance and provides better control over MXenes synthesis, offering new possibilities and insights for future applications.

# AlGaN buffer layers grown on sapphire substrates

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Keywords: MOVPE, AlGaN, UV LED

Growing AlGaN directly on sapphire has been identified as a niche area of research, since most applications involving AlGaN material can rely on a growth of binary compounds (GaN or AlN) as a nucleation and buffer layers. GaN has been identified as an optimal buffer layer for most of UVA emitters, however, with increasing Al content and layer thickness of AlGaN grown on top of GaN, the layers become susceptible to cracking due to a tensile strain. It is therefore technically relevant to manufacture light sources down to around 340 nm of emission wavelength. The employment of AlN as a buffer layer is beneficial for UVC and UVB range, and the utilization of AlN in UVB up to around 310 nm of emission wavelength was published [1]. This leads to a known gap with low external quantum efficiency (EQE) in the emission region 310-340 nm, as reported in [2].

In order to enhance EQE in the region of 340 to 310 nm, we propose the process of growing high quality AlGaN buffer directly on sapphire substrate. This process is generally considered as very difficult, due to the different Al and Ga adatom mobility causing phase separations and the emergence of defects [3]. This contribution will discuss a series of AlGaN buffers grown on sapphire using thin GaN nucleation, with concentration of Al of around 30%. Different growth process parameters will be discussed regarding the solid-state Al: Ga ratio, surface quality with regard to the "pancake defects" [4] and threading dislocation density. These are evaluated via Raman spectroscopy, photoluminescence, scanning electron microscopy, etch pit density, and X-ray diffraction.

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# Thick InGaN layers for water photocatalysis grown on sapphire substrate by MOVPE

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Keywords: InGaN layer, photocatalysis, green hydrogen generation

The demand for hydrogen generation is rising steadily, and it is expected to increase exponentially from 2035 onwards, reaching 150 to 500 million metric tons per year by 2050 [1]. However, current technological processes are mainly grey energy production, which is not environmentally sustainable for such high expected demands. Consequently, there is an ongoing search for a green and efficient source of hydrogen. InGaN has recently been identified as a very promising material for photocatalysis (PC) of water to obtain green hydrogen [2]. The potential of the InGaN material lies in its band gap tunability which can be tailored to match the redox potential of water. A notable advantage of InGaN is also its relatively small band gap, which is advantageous compared to other semiconductors used in PC, such as $TiO_2$ or ZnO, because it allows PC process to be powered by major part of sun instead of an artificial UV source; a factor crucial for sustainability. Utilization of pure water avoids the need for an aggressive and potentially harmful electrolyte which also increases the device lifetime and long-term stability.

The InGaN layers were prepared by Metalorganic Vapor Phase Epitaxy directly on sapphire substrates with no buffer layers. Since the lattice mismatch for sapphire and InGaN is high, a series of nucleation layers was tested, and the growth parameters like precursor flow, growth temperature and showerhead gap were varied. This methodical approach enabled the preparation of InGaN layers with thicknesses up to 1 µm. The quality of the layers was investigated using a scanning electron microscope, and further evaluation was conducted via photoluminescence and X-ray diffraction measurements. Plans for sample processing to produce a final device with enlarged surface will also be presented.

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# Fully digital 3D imager for hard X-rays: MBE growth and fabrication challenges

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Keywords: Avalanche Photo Diode, Hard X-rays, GaAs/AlGaAs

Time-resolved, ultrafast phenomena with radiation from hard-X to gamma-rays are one of the groundbreaking research fields at the base of scientific and medical applications like pump-and-probe spectroscopy and Time-of-Flight Positron Emission Tomography.

GaAs, thanks to its higher atomic number and mobility, has the potential to be much more efficient and faster than silicon in absorbing hard X-rays. Coupled with cross-delay lines and a high-precision time-to-digital converters, we aim at a realizing a ~1cm2 detector with 2D spatial and temporal precision of 100 µm and 10 ps, respectively.

MBE growth of the p-, absorption, multiplication, and n- layers will be reported along with the subsequent fabrication steps. The fine tuning of the doping levels of the p- and n-layers and the tailoring of the multiplication region based on simulations will be described. Special attention will be devoted to the various fabrication steps leading to the final device, along with their optimization.

The authors acknowledge the financial support from Italian MIUR through PRIN 20227N9LW7.

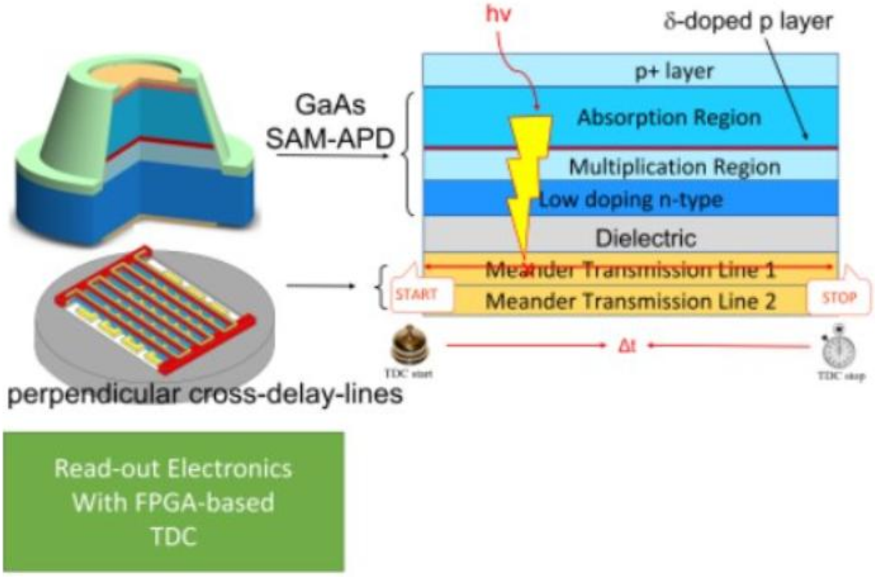

Fig.1. A sketch of the complete device along with a schematic cross section of the active region

# Epitaxial Growth of Iron and Cobalt on Oxide Substrates

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Keywords: Molecular Beam Epitaxy, Low Energy Electron Diffraction, X-Ray Photoelectron Spectroscopy

Molecular beam epitaxy (MBE) is a highly precise technique for the deposition of thin films, enabling the controlled layer-by-layer growth of materials with atomic-level precision under ultra-high vacuum conditions. MBE facilitates epitaxial alignment between the deposited film and the substrate, making it a pivotal method for fabricating advanced heterostructures such as GaAs/AlGaAs and GaN/AlBaN, which are essential for optoelectronic devices and high-performance transistors. The precise control offered by MBE enables the tailoring of layer compositions and thicknesses at the atomic scale, allowing for the optimization of electronic properties and quantum effects in advanced semiconductor applications. Despite its remarkable precision, molecular beam epitaxy faces challenges such as maintaining ultra-high vacuum conditions and controlling the purity of source materials, both of which are critical for achieving defect-free heterostructures. Additionally, the complexity of managing interfacial strain and lattice mismatches between layers limits the range of compatible substrate-material combinations, posing further obstacles to optimizing the performance of electronic devices. Here, we report a new, easier method to grow transition metals on oxides from oxyhydroxides precursors. Focusing on FeOOH and CoOOH deposited by chemical methods on SrTiO3 (STO) substrates, we achieve epitaxial Fe and Co layers by series of flash annealing. The resulting films exhibit remarkable surface crystallinity, as evidenced by the high-quality LEED patterns shown below.
Our newly developed technique could be easily extended to other materials and substrates.

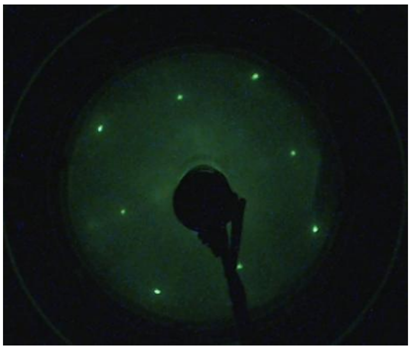

*Figure 1 Fe on STO(001)*

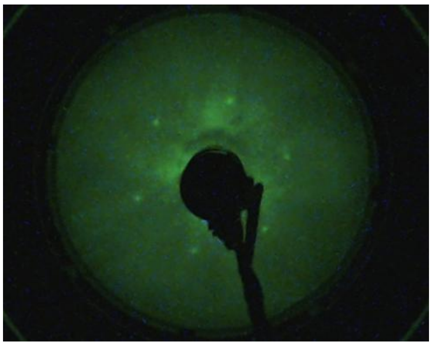

*Figure 2 Fe on STO(111)*

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**PS.18**

# SiGe PIC sensor

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Keywords: epitaxy, intersubband transiBons, quantum wells infrared photodetectors, nextnano

Photonic integrated circuits (PICs) operating in the mid-infrared (4 -14 µm) are receiving increasing attention due to the variety of applications envisaged in medical diagnosis, analytical chemistry, environmental monitoring, and sensing for safety and security. In the MIR, molecules exhibit unique and spectrally narrow vibrational bands. The architecture of PIC sensors is typically based on the evanescent field at the interface between the volume occupied by the target analyzer and a layer of waveguide material. At wavelengths below 4 µm, MIR PICs can be designed on the standard siliconon- insulator (SOI) platform, but multi-phonon and polar-phonon absorption hinder their use at longer wavelengths, where several material platforms with extended transparency (including SiGe) are under investigation. Confinement and guiding of optical modes in the MIR can be achieved by the transparency of semiconductors in this spectral range. For this purpose, rib or ridged waveguides are typically etched from a thin semiconductor layer, grown epitaxically on a lower refractive index substrate, thus confining the radiation to the higher region. Recently there was an intense research effort aimed at developing thin films suitable for the realization of MIR WGs based on material platforms characterized by high transparency in the entire MIR range, such as those based on chalcogenide glasses, III-V semiconductors , SiGe with high Ge content [1], and pure Ge [2]. PIC approaches based on silicon foundry-friendly materials such as SiGe alloys are to be preferred [3]. Another relevant advantage of this material system is represented by its potential to integrate the waveguide functionalities with Ge/SiGe or Si/SiGe integrated quantum well infrared photodetectors (QWIPs). QWIPs are unipolar detectors in which the photocurrent is related to the excitation of intersubband transitions (ISBTs) in quantum wells (QWs) formed in the conduction band (n-type) or valence band (p-type) of multilayer heterostructures. Waveguide-integrated QWIPs in PICs have been rarely studied. SiGe QWIP integration into PICs would enable full automation of a new class of compact and affordable molecular sensing systems with resounding advancements in a number of applicative contexts. The final aim of our project is to engineer a photonic chip for MIR sensing, made of SiGe epitaxial layers grown on a Si substrate, realized integrating WGs and quantum well infrared photodetectors and to test it by means of sensing experiments with CH4. The heterostructure investigated in this project features a 3-nm thick Ge quantum well doped with holes sandwiched between 8-nm thick barriers coherently grown on a VS (virtual substrates). The choice of a hole-based heterostructure is motivated by the larger offsets, up to 300 meV, occurring in the valence band of Ge/SiGe QWs, as required to design ISBTs falling in the MIR spectral range, whereas those occurring in the conduction band and specifically in the L-valley are limited to 100-150 meV, making them suitable for far- infrared applications. The Ge/SiGe QWs benefit from the lower effective mass of the heavy holes in Ge (0.33 me) compared to that of Si (0.49 me), allowing ISBT with a superior oscillator strength compared to the Si/SiGe QWs. The electronic band structure of the system was calculated using a self-consistent multivalley Schro d̈ inger-Poisson solver based on a tightbinding first-neighbor semiempirical Hamiltonian model including the spin-orbit interaction and taking into account the strong nonparabolicity and band mixing that typically occur in the valence band, my work has been to calcute the band structure with the Nextnano software [4,5], a software for semiconductor nanodevices with which the transport of charges, in our case the holes, will then be calculated. Opposed to the many commercial semiconductor simulation tools that treat quantum mechanical effects as perturbations, Nextnano focuses on nanostructures where quantum mechanical effects such as electronic band structures, optical matrix elements, magnetic field effects, or tunneling effects play a vital role. Using an extensive materials database for Si/Ge and III-V materials including nitride semiconductors, their binary, ternary, and quaternary alloys, and both zincblende and wurtzite crystal structures, a wide

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variety of quantum structures can be modeled with almost arbitrary device geometries. Since most nanostructures are strained materials, nextnano performs a global strain minimization based on macroscopic elasticity theory. Once the strain field has been calculated, the piezoelectric and (for wurtzite) pyroelectric charges are determined. Then the electronic structure is calculated within a multi- band k · p envelope function approximation. Here, exchange-correlation effects are taken into account through the local density approximation and the Hartree electron-electron interaction by self-consistently solving the Poisson equation. Additionally, the spin-orbit interaction and the Zeeman term are also included to handle spin and magnetic field effects. Interband and intraband optical transition matrix elements between electron and hole wave- functions can also be computed. All of the above features deal with equilibrium systems. Therefore, in order to enable the simulation of nanodevice properties under applied bias, nextnano also includes two models for the carrier transport. One is a WKB (Wentzel-Kramers- Brillouin) approach applied to drift-diffusion method, where we assume that the carriers are locally in equilibrium, characterized by a local Fermi level. The other approach, called the contact block reduction method (CBR), is based on an efficient method to calculate the ballistic current through an open system of arbitrary shape with any number of conductors.

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# Unexpected trench self-patterning in InGaAs/InP: a route to pseudo-substrates for 2 µm applications

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Keywords: MOVPE, InGaAs, tensile strain, pseudomorphic, trench

III-V semiconductors are key materials for opto-electronic applications due to their broad heteroepitaxial wavelength tunability. Despite the far-reaching developments of planar devices across many fields, some wavelengths are still challenging to reach while keeping good material quality. In particular, long range wavelength (> 2 µm) devices on conventional substrate (InP) require highly lattice-mismatched heterostructures. This leads to high strain in the active region, inducing interface defects, threading dislocations, wafer bowing and while also limiting the design to thin layers. These limitations are even more dramatic for applications where thick layers are needed and more generally for complex integrated devices. Whilst many workarounds for strain management have been developed over the years the challenges persist and not all issues are effectively solved.

Here, we present a new and unreported growth process by metalorganic vapour phase epitaxy (MOVPE) of crystallographic trench self-patterning in InP heterostructures. Importantly, this approach does not exhibit the apparent creation of other defects. We observe the formation of perpendicular trench arrays (i.e. cracks along the cleavage directions, <110>) in an InGaAs highly tensile layer, which propagates in the InP substrate underneath (see Fig. 1). Surprisingly, under our growth conditions, the highly tensile InGaAs areas between the trenches, are pseudomorphic, "defect-free" and exhibit a smooth surface morphology even for relatively thick layers (hundreds of nm). In comparison, compressive strain would allow only a few nm coherent InGaAs layer at equivalent strain modulus [1]. To note that a similar tensile strain relaxation process ("cracks") was reported in the literature in the early 90s but was always accompanied with a high defect density and wavy surface organisation [2].

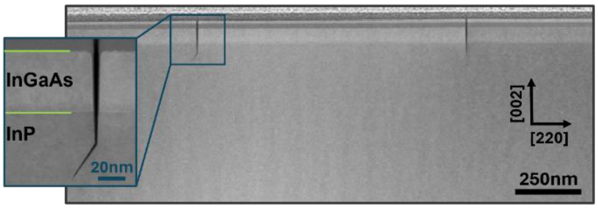

*Fig. 1 : HAADF- STEM image of the highly tensile InGaAs layer grow on InP substrate.*

An interesting aspect of this pseudo-substrate is the possible compliant capacity to release high strain through deformation of the trench free-surface, compare to a rigid bulk substrate, while not affecting the defect-free area. From our preliminary studies, for example, we compared the growth of ten highly strain-balanced quantum wells, emitting around 2 µm at room temperature, on standard bulk substrate and on this trench buffer. Structural characterization by AFM and XRD indicated that the trench buffer structure displays better surface morphology with no additional defects. The comparable optical properties of the two structures, suggests that the trench does not have any drawback effect on the area in-between.

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Pisa, May 2025

# $MoS_2/PtX_2$ van der Waals heterostructures

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Keywords: 2D heterostructures, $MoS_2$, $PtSe_2$, $PtTe_2$

Van der Waals engineering, the construction of van der Waals heterostructure by arbitrarily stacking of two or more 2D materials bound with interlayer van der Waals force, provides a convenient way to further alter their properties. 2D $MoS_2$, $PtSe_2$ and $PtTe_2$ are all synthesized on sapphire substrates by CVD technique. For heterostructures vertical stacking $MoS_2$ thin films were transferred from sapphire substrates onto different transition metal dichalcogenide (TMDC) layers using a PMMA-assisted process. The formed $MoS_2/PtSe_2$ and $MoS_2/PtTe_2$ heterostructures are studied by room temperature Raman spectroscopy (Fig.1 and Fig2.), photoluminescence and XPS. Vertical stacking of TMDC materials can lead to a wide variety of new heterostructure materials, where layered materials are held by weak van der Waals (vdW) forces. These 2D vdW heterostructures offer a great promise for creating new functional material platforms for high-performance or emerging devices.

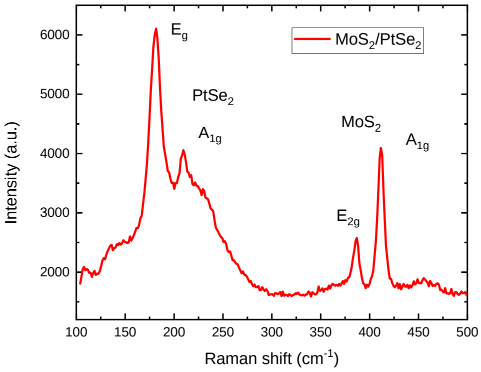

Fig.1. Raman spectroscopy of $MoS_2/PtSe_2$ heterostructure

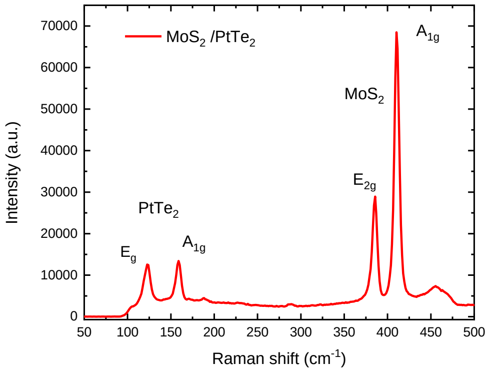

Fig.2. Raman spectroscopy of $MoS_2/PtTe_2$ heterostructure

Acknowledgement: This work was supported by the Bulgarian Science Fund under the grant number КП- 06-COST/15 under the COST CA 20116 Action “European Network for Innovative and Advanced Epitaxy” (OPERA).

# Pt- and Pd- based noble-metal dichalcogenides

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Keywords: 2D, Noble-metal dichalcogenides, Thermally Assisted Conversion method, self-flux method

Noble-metal dichalcogenides (NMDs) have attracted significant attention as new members of the 2D material family due to their layer-controllable metal-to-semiconductor transition. Both few-layer and bulk phases exhibit the topological properties of Dirac type-II semimetals [1]. Additionally, NMDs have demonstrated outstanding performance in opto-electronics and photonics as photo detectors, transistors, sensors, super-capacitors, in biomedicine, etc. [2]. Their unique chemistry—characterized by highly anisotropic structural features, low-energy differences between polymorphs, controllable phase changes, and catalytic properties sets them apart from other transition-metal dichalcogenides [2].

Thermally Assisted Conversion (TAC), has been employed for the synthesis of 2D $PtSe_2$ nanolayers [3]. This method is notable for its relatively low growth temperature and the production of polycrystalline $PtSe_2$ films with nanometer-sized grains. Integration of $PtSe_2$ as transparent, conductive layers in Polymer Dispersed Liquid Crystal (PDLC) structures, functioning as near-infrared light shutters, has been demonstrated [5].

$PdSe_2$ single crystals have been successfully obtained using a self-flux method [4]. The structural, chemical, optical, and electrical properties of $PtSe_2$ and $PdSe_2$ have been thoroughly investigated using techniques such as XRD, XPS, AFM, Raman spectroscopy, ellipsometry, spectrophotometry, and Hall effect measurements. It was found that pentagonal $PdSe_2$, characterized by unique in-plane anisotropy, induces unprecedented gate-tunable spin-orbit coupling (SOC) in graphene [6]. In addition, PdSe2 -based photodiode device will be demonstrated.

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# Transmission Electron Microscopy Analysis of $Ga_2O_3$ Thin Films Homoepitaxially Grown on (010), (-201) and (001) Substrates

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Keywords: Epitaxy, MOVPE (MOCVD), Ga2O3 semiconductors, transmission electron microscopy.

β-Ga2O3 epilayers were grown simultaneously on (010), (-201), and (001) oriented Ga2O3 substrates by Metal-Organic Vapor Phase Epitaxy (MOVPE). The crystalline structure of these homoepitaxial films was characterized with atomic scale resolution by using high angle annular dark field (HAADF) scanning transmission electron microscopy (STEM, ThermoFisher Spectra microscope operating at 300 kV). The system includes energy dispersive X-ray spectroscopy (EDS) enabling chemical analysis and mapping. The images in the figure below reveal that homoepitaxial growth on (010) occurred without generation of extended defects or dislocations. For this (010) orientation, STEM was performed across [001] zone axis and we remark the occurrence of additional contrasts between two Ga1 atomic columns, as indicated by the blue arrow in the insert of figure (c), which we attributed to columns of interstitial Ga, as suggested in reference [1]. Results are also given on homoepitaxies carried out on (-201) orientation, where V-shape defects have been characterized, and on (001) orientation which shows more pronounced heterogeneity.

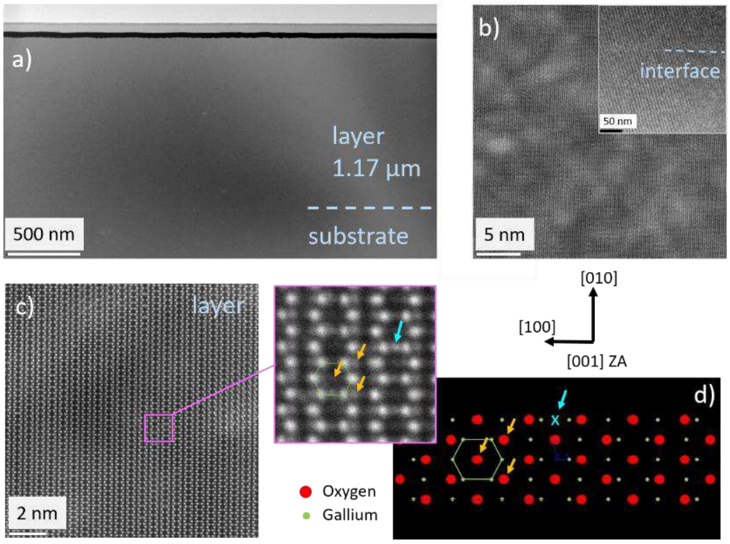

Figure : STEM analysis of a Ga2O3 epilayer grown on (010) Ga2O3 substrate, with [001] zone axis

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# MOCVD growth of $Zn_xCd_{(1-x)}S$ epilayers on non-polar m-plane and a-plane wurtzite CdS substrates

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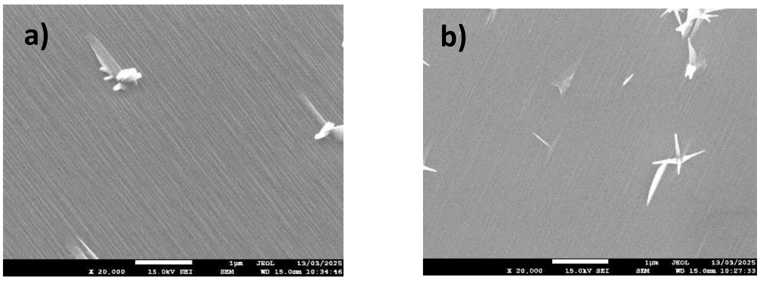
Keywords: Epitaxy, MOCVD, II-VI semiconductors, ZnCdS ternary alloy, CdS substrate

The results that are reported here are part of the ANR ADHEX-SiGe project. The aim is to advance the integration of SiGe materials with direct bandgap for a new generation of optoelectronic devices. It focuses on developing innovative approaches to achieve SiGe epilayers with hexagonal symmetry. One of the proposed solutions is to grow a wurtzite (WZ) ZnCdS buffer layer in order to reduce the lattice mismatch and enable the best quality of WZ-SiGe layer.

This study focuses on the growth of the $Zn_xCd_{(1-x)}S$ buffer layers on non-polar m-plane and a-plane wurtzite CdS substrates. The process involves cleaning of substrate surface, followed by ternary alloy deposition via MOCVD using DTBS, DMCd and DEZn precursors under atmospheric pressure. The substrates are first annealed at 500°C during 5 minutes under N2 flux. Then the growth is carried out at 360°C for 15 min. The morphology and crystal structure are examined by scanning electron microscopy (SEM) and X-ray diffraction (XRD).

As shown in the SEM pictures below, despite some structural defects, CdS layer grown on m-plane and a-plane substrates is relatively smooth. As the Zn content increases, the defects density is higher and the surface of the layers becomes rougher. From composition x=0.4, cracks appear on the surface of the layer.

XRD experiments indicate that ZnCdS layers grown on m-plane CdS substrate crystalize in a wurtzite structure. A series of X-ray diffraction patterns of ZnCdS alloys grown on m-plane substrate with different Cd composition shows a shift of the peak associated to the layer as the Zn composition increases. However, no peak from the layer grown on a-plane substrate is observed. Further investigations are needed to identify the detailed crystal structure of the layers and understand these preliminary results.



CdS layers grown by MOCVD at 360°C on (a) m-plane and (b) a-plane CdS substrate

**PS.24**

# Ge and GeSn NWs for group IV Photonic applications

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Silicon is an ideal material for waveguiding in the near IR (NIR) and light detection in the visible light spectrum (VIS). However, due to its indirect bandgap, it is unsuitable for light emission. The current approach is to use Si for light transmission and integrate active optical devices with compound semiconductors (III-Vs). The aim of this project is the development of a semiconductor platform based on high-quality $Si_xGe_{1-x}$ and $Ge_{1-y}Sn_y$, enabling active optoelectronic devices CMOS compatible with reduced environmental impact compared to compound semiconductors III-Vs. To do so, we are investigating bottom-up approaches based on the SAE (Selective Area Epitaxy) and TASE (Template Assisted Selective epitaxy) of Ge nanowires by MOVPE. These techniques allow to selectively grow single crystalline heterostructures.

Ge NWs growth by SAE through MOVPE has already demonstrated successful results [1]. This process consists on pattern desired openings on a $SiO_2$ mask deposited on a Si substrate. To achieve the epitaxial growth of Ge NWs on Si, remove the native oxide on the openings is needed. the substrate undergoes a deoxidation process on the reactor for surface preparation, using a AsH3 atmosphere before the growth.

However, the use of $AsH_3$ for native oxide removal, induces As impurities on the Ge NWs, which are detrimental for quantum applications. To further improve crystalline quality and purity, as well as improving the sustainability of the whole process, the use of $AsH_3$ for oxide removal is substituted by a catalysed $H_2$ in situ anneal.

Another alternative to achieve high quality Ge NWs on Si has been explored. TASE technique consists on bury a Si nanostructure on $SiO_2$ [2]. Through an opening on the $SiO_2$ mask, the Si nanostructure is etched down until a small portion of Si remains to act as a seed for the Ge growth by MOVPE along the nanohollow.

Advantages of the TASE growth includes integration of heterojunctions and doping profiles in-situ and in-plane along the surface of the substrate, which facilitates the fabrication of advanced electronic or optoelectronic devices.

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