European Network for Innovative and Advanced Epitaxy "OPERA" COST Action

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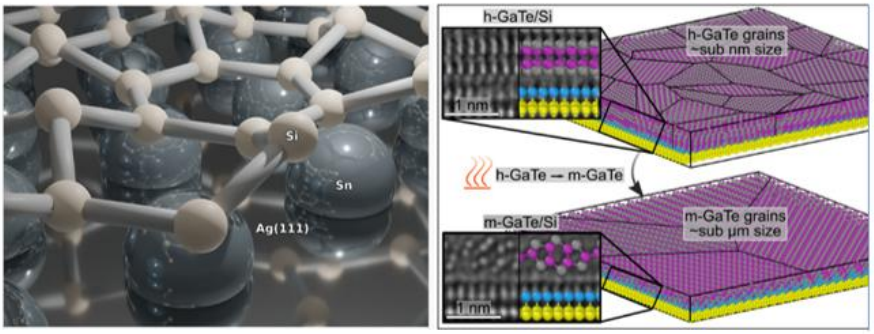
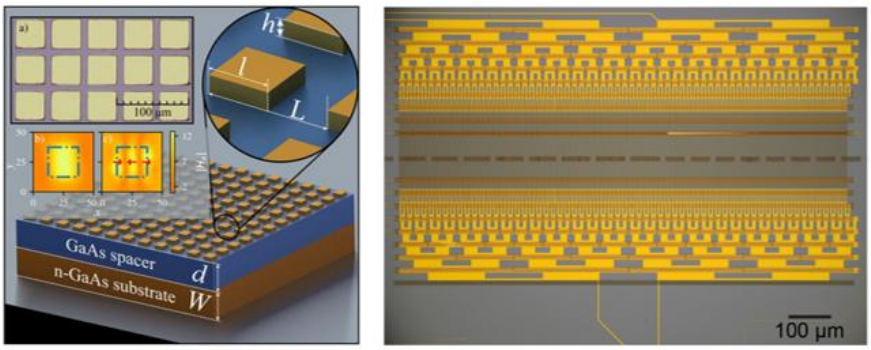
COST Action CA20116

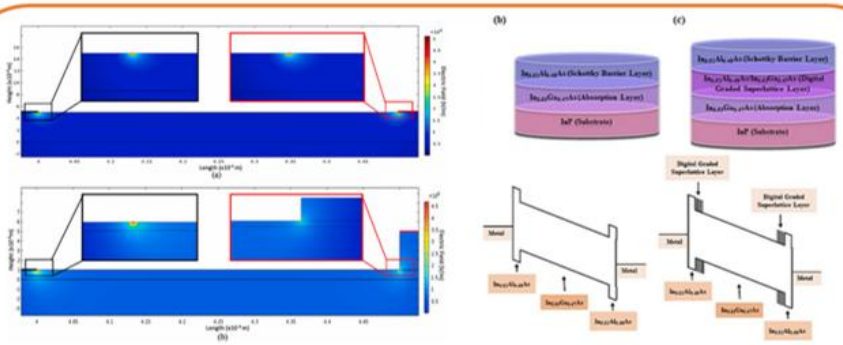
# Highlights 2023




WG 1: Fundamental research – New Materials




WG 2: Applications-oriented material developments



WG 3: Industry-oriented materials development and technological transfers

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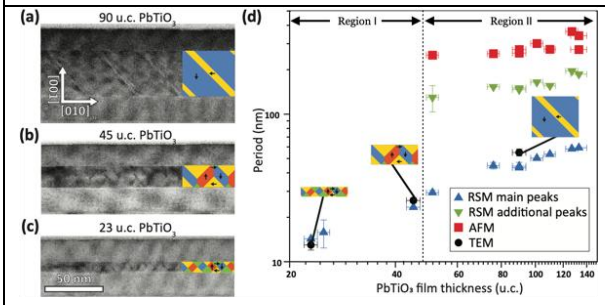
# I- Fundamental research – New Materials (WG1)

## Mapping the complex evolution of ferroelastic/ferroelectric domain patterns in epitaxially strained $PbTiO_3$ heterostructures




*Reference:* *APL Mater. 1 June 2023; 11 (6): 061126. https://doi.org/10.1063/5.0154161*

*Authors:* *C. Lichtensteiger, M. Hadjimichael, E. Zatterin, C.-P. Su, I. Gaponenko, L. Tovaglieri, P. Paruch, A. Gloter, J.-M. Triscone*

*Laboratories:* *UniGe(CH), ESRF(Fr), CNRS(Fr)*

*Techniques:* *sputtering, AFM, XRD, TEM*

*Materials:* *$PbTiO_3$, $SrRuO_3$, $DyScO_3$*

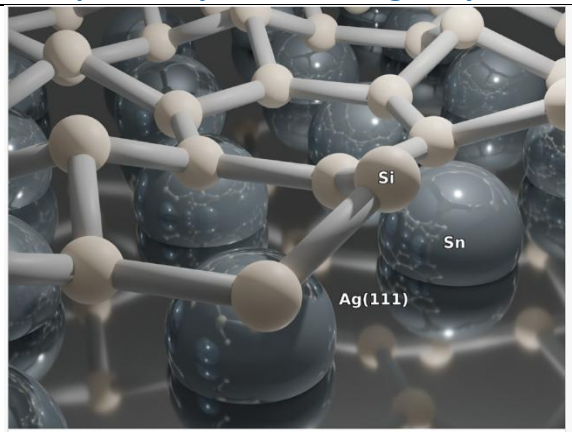

### Abstract

*We study the complex ferroelastic/ferroelectric domain structure in the prototypical ferroelectric $PbTiO_3$ epitaxially strained on $(110)_o$-oriented $DyScO_3$ substrates, using a combination of atomic force microscopy, laboratory and synchrotron x-ray diffraction and high resolution scanning transmission electron microscopy. We observe that the anisotropic strain imposed by the orthorhombic substrate creates a large asymmetry in the domain configuration, with domain walls macroscopically aligned along one of the two in-plane directions. We show that the periodicity as a function of film thickness deviates from the Kittel law. As the ferroelectric film thickness increases, we find that the domain configuration evolves from flux-closure to a/c-phase, with a larger scale arrangement of domains into superdomains.*


### OPERA Work Group

*WG1*

## Epitaxial Synthesis of Single Crystal Silicene onto Sn-Engineered Ag(111) Templates




*Reference:* *Nanoscale 15, 11005 (2023); DOI: 10.1039/D3NR01581E*

*Authors:* *S. Achilli, D. S. Dhungana, F. Orlando, C. Grazianetti, C. Martella, A. Molle, G. Fratesi*

*Laboratories:* *CNR-IMM (It), Univ. Milano (It)*

*Techniques:* *MBE, Raman Spectroscopy, DFT*

*Materials:* *Silicene, Stanene*

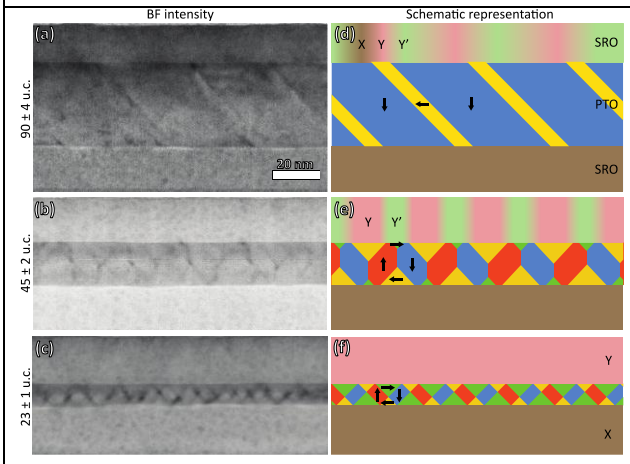

### Abstract

*The synthesis of silicene by direct growth on silver is characterized by the formation of multiple phases and domains, posing severe constraints on the spatial charge conduction towards a technological transfer of silicene to electronic transport devices. Here we engineer the silicene/silver interface by two schemes, namely, either through decoration by Sn atoms, forming an $Ag_2Sn$ surface alloy, or by buffering the interface with a stanene layer. Whereas in both cases Raman spectra confirm the typical features as expected from silicene, by electron diffraction we observe that a very well-ordered single-phase 4 × 4 monolayer silicene is stabilized by the decorated surface, while the buffered interface exhibits a sharp √3 × √3 phase at all silicon coverages. Both interfaces also stabilize the ordered growth of a √3 × √3 phase in the multilayer range, featuring a single rotational domain. Theoretical ab initio models are used to investigate low-buckled silicene phases (4 × 4 and a competing √13 × √13) and various √3 × √3 structures, supporting the experimental findings. This study provides new and promising technology routes to manipulate the silicene structure by controlled phase selection and single-crystal silicene growth on a wafer-scale.*


### OPERA Work Group

*WG1*

## Nanoscale domain engineering in $SrRuO_3$ thin films




*Reference:* *APL Mater. 1 October 2023; 11 (10): 101110. https://doi.org/10.1063/5.0167553*

*Authors:* *C. Lichtensteiger, C.-P. Su, I. Gaponenko, M. Hadjimichael, L. Tovaglieri, P. Paruch, A. Gloter, J.-M. Triscone*

*Laboratories:* *UniGe(CH), CNRS(Fr)*

*Techniques:* *sputtering, AFM, XRD, TEM, GPA*

*Materials:* *$SrRuO_3$, $PbTiO_3$, $DyScO_3$*

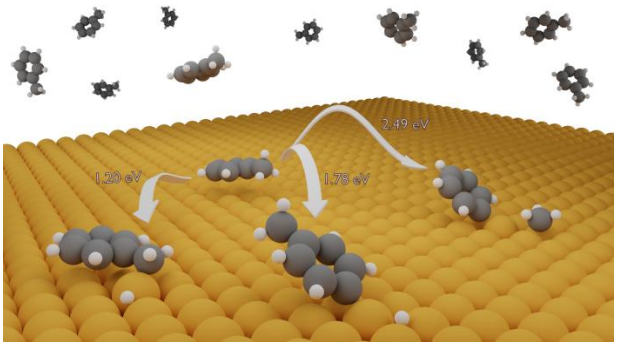

### Abstract

*We investigate nanoscale domain engineering via epitaxial coupling in a set of $SrRuO_3/PbTiO_3/SrRuO_3$ heterostructures epitaxially grown on (110)o-oriented $DyScO_3$ substrates. The $SrRuO_3$ layer thickness is kept at 55 unit cells, whereas the $PbTiO_3$ layer is grown to thicknesses of 23, 45, and 90 unit cells. Through a combination of atomic force microscopy, x-ray diffraction, and high resolution scanning transmission electron microscopy studies, we find that above a certain critical thickness of the ferroelectric layer, the large structural distortions associated with the ferroelastic domains propagate through the top $SrRuO_3$ layer, locally modifying the orientation of the orthorhombic $SrRuO_3$ and creating a modulated structure that extends beyond the ferroelectric layer boundaries.*


### OPERA Work Group

*WG1*

## Adsorption and decomposition steps on Cu(111) of liquid aromatic hydrocarbon precursors for low-temperature CVD of graphene: A DFT study




*Reference:* *Carbon 206 (2023) 142–149 ; DOI: 10.1016/j.carbon.2023.02.011*

*Authors:*, *O. Tau , N. Lovergine, P. Prete*

*Laboratories:* *IMM-CNR (It), Univ. Salento (It)*

*Techniques:* *DFT simulations.*

*Materials:* *Cu(111), aromatic hydorcarbons*

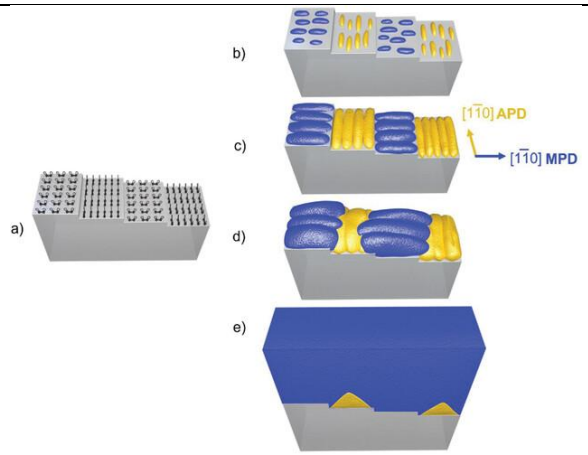

### Abstract

*Low-temperature chemical vapor deposition (LT-CVD) of graphene using liquid aromatic hydrocarbons holds technological advantages over conventional growth from methane. However, the nature of decomposition mechanisms of such precursors and their effectiveness in a LT-CVD process is still debated. We investigate by means of density functional theory adsorption energies and decomposition first steps on Cu(111) of single-ring aromatic hydrocarbons, such as benzene and toluene. Our results confirm the stronger stability with respect to methane of aromatic adsorbates, due to exchange of London dispersion forces with Cu surface; however, toluene exhibits improved bindings with respect to benzene. The adsorption energy slightly improves if additional methyl groups are substituted in benzene, as in o-xylene and 1,2,3-trimethylbenzene. Among decomposition reactions, dehydrogenation of the methyl group in toluene is energetically more favored (1.20 eV) than that of methane (1.52 eV) or aromatic C-rings (1.67 eV and 1.72 eV for benzene and toluene), while demethylation of toluene remains negligible due to the prohibitive energy barrier (2.49 eV). Methyl dehydrogenation in toluene leads to the abundant formation of adsorbed benzyl radicals onto Cu in an almost parallel-to-surface configuration, as active species for graphene nucleation. Toluene (and to a lesser extent o-xylene and 1,2,3-trimethylbenzene) should be thus preferred to benzene in the LT-CVD of graphene*


### OPERA Work Group

*WG1*

## Epitaxial Growth of III-Vs on On-Axis Si: Breaking the Symmetry for Antiphase Domains Control and Burying




*Reference:* *Adv. Optical Mater. 11, 2203050 (2023); DOI: https://doi.org/10.1002/adom.202203050*

*Authors:* *A. Gilbert, M. Ramonda, L. Cerutti, C. Cornet, G. Patriarche, É. Tournié, J.-B. Rodriguez.*

*Laboratories:* *IES (fr), Institut FOTON (fr), C2N (fr).*

*Techniques:* *MBE, AFM, TEM.*

*Materials:* *GaAs/Si*

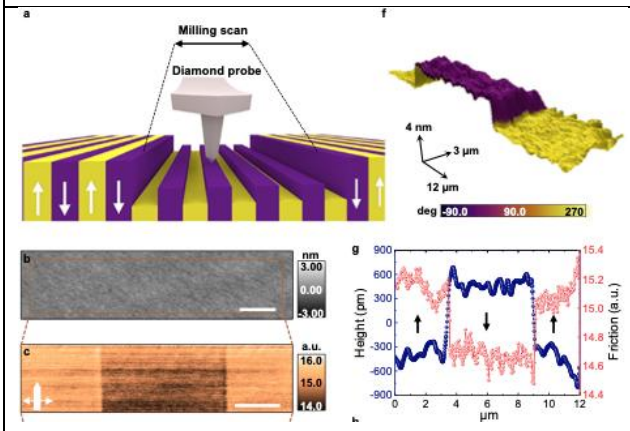

### Abstract

*This work reports on the precise control of III-V semiconductors' antiphase domain formation and evolution during the epitaxial growth on an "on-axis" Si (001) substrate with a very low but controlled miscut. Especially, it is shown how, starting from a Si surface having a regular array of terraces, the crystal polarity of thin GaAs epilayers grown by molecular-beam epitaxy is defined through the Si surface topology, leading to a quasi-periodic 1D pattern of antiphase domains in the GaAs layer. Furthermore, this work demonstrates how this configuration breaks the symmetry between the two different III-V phases, without any step-flow-induced asymmetry. Following this strategy, an early burying of antiphase domains is demonstrated in GaAs epitaxially grown on a low-miscut Si substrate. This study generalizes previous models describing antiphase domain formation and evolution and establishes the important growth parameters for the development of high crystal quality III-V semiconductor devices monolithically integrated on low-miscut silicon substrates.*


### OPERA Work Group

*WG1*

## Switchable tribology of ferroelectrics




*Reference:* *Nat Commun **15**, 387 (2024). https://doi.org/10.1038/s41467-023-44346-0*

*Authors:* *S. Cho, I. Gaponenko, K. Cordero-Edwards, J. Barceló-Mercader, I. Arias, D. Kim, C. Lichtensteiger, J. Yeom, L. Musy, H. Kim, S. Min Han, G. Catalan, P. Paruch & S. Hong*

*Laboratories:* *KAIST (Republic of Korea), UniGe(CH), LaCàN (Spain), CIMNE(Spain), ICN2(Spain), ICREA(Spain)*

*Techniques:* *SPM, lithography*

*Materials:* *PPLN, PZN-5.5%PT, $PbTiO_3$, $LiNbO_3$*

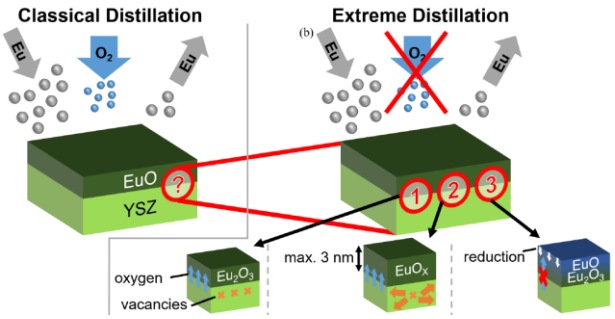

### Abstract

*Artificially induced asymmetric tribological properties of ferroelectrics offer an alternative route to visualize and control ferroelectric domains. Here, we observe the switchable friction and wear behavior of ferroelectrics using a nanoscale scanning probe where down domains having lower friction coefficient than up domains can be used as smart masks as they show slower wear rate than up domains. This asymmetry is enabled by flexoelectrically coupled polarization in the up and down domains under a sufficiently high contact force. Moreover, we determine that this polarization-sensitive tribological asymmetry is universal across ferroelectrics with different chemical composition and crystalline symmetry. Finally, using this switchable tribology and multi-pass patterning with a domain-based dynamic smart mask, we demonstrate three-dimensional nanostructuring exploiting the asymmetric wear rates of up and down domains, which can, furthermore, be scaled up to technologically relevant (mm-cm) size. These findings establish that ferroelectrics are electrically tunable tribological materials at the nanoscale for versatile applications.*


### OPERA Work Group

*WG1*

## Europium oxide: Growth guide for the first monolayers on oxidic substrates




*Reference:* *Phys. Rev. Materials* ***6***, *044404 (2022) - DOI: 10.1103/PhysRevMaterials.6.044404*

*Authors:* *P. Rosenberger and M. Müller*

*Laboratories:* *University of Konstanz (D),*

*Techniques:* *MBE, XPS, LEED*

*Materials:* *Europium Monoxide (EuO), YSZ*

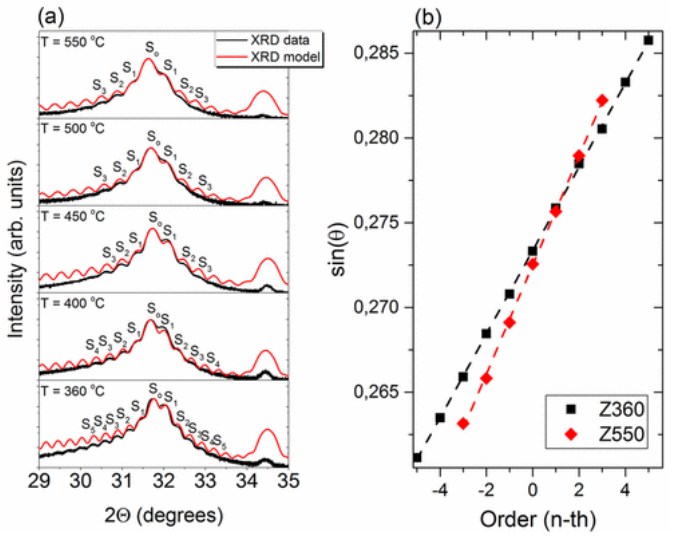
### *Abstract*

*Interfacial oxygen exchange at oxide interfaces bears huge potential in stabilizing metastable or novelphases of functional oxides down to the monolayer limit. By taking advantage of active oxygen supply of the substrate material, waiving any external oxygen dosage, high-quality, crystalline ultrathin films of the Heisenberg ferromagnet europium monoxide (EuO) were stabilized on YSZ (001). This so-called redox-assisted growth mode (or, vice versa, the extreme case of a distillation growth) was monitored end to end by in situ x-ray photoelectron emission spectroscopy and electron diffraction techniques. The evolution of Eu 3d core levels allows us to disentangle the processes of interfacial oxygen diffusion and vacancy formation in stabilizing the very first monolayers of EuO on YSZ (001). We concluded on the key mechanisms of redox-assisted EuO/YSZ (001) thin film synthesis, which merge in a universal three-process growth model that may serve as guideline for redox-assisted synthesis of metastable low-dimensional oxides.*

### *OPERA Work Group*

*WG1*

## The Influence of the Growth Temperature on the Structural Properties of $\{CdO/ZnO\}_{30}$ Superlattices




*Reference:* *Cryst. Growth Des. 2023, 23, 1, 134–141; DOI: https://doi.org/10.1021/acs.cgd.2c00826*

*Authors:* *A. Lysak, E. Przeździecka, A. Wierzbicka, P. Dłużewski, J. Sajkowski, K. Morawiec, and A. Kozanecki*

*Laboratories:* *Institute of Physics, Polish Academy of Sciences (Pl)*

*Techniques:* *PA-MBE.*

*Materials:* *CdO/ZnO Superlattices*

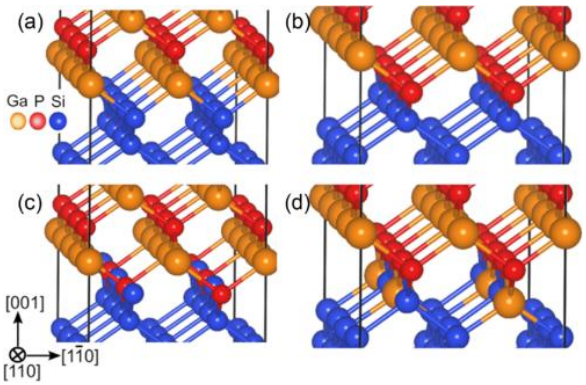
### *Abstract*

*The {ZnO/CdO}30 superlattices (SLs) series were grown at different temperatures (350–550 °C) on m-plane $Al_2O_3$ substrates by molecular beam epitaxy. The structural properties of SLs were investigated using high resolution XRD and TEM methods. The periodic structure of the obtained {ZnO/CdO}30 SLs was confirmed by cross-sectional TEM images. Satellite peaks (S1, S2, S3...) surrounding the main zero-order peak (S0) and characteristic of the periodic superlattice structure were found in the X-ray analysis. X'Pert Epitaxy software was used to simulate the XRD data to determine the ZnO and CdO sublayers thicknesses and the SLs period. It was found that growth at relatively low temperatures is favorable for the quality of the superlattices. The thicknesses of the ZnO and CdO sublayers change with growth temperature. Some deterioration of the {ZnO/CdO}30 structure quality and changes in the period of the superlattices were also confirmed by TEM analysis.*

### *OPERA Work Group*

*WG1*

## Determination of III-V/Si absolute interface energies: Impact on wetting properties




*Reference:* *Phys. Rev. B 108, 075305 (2023); DOI: https://doi.org/10.1103/PhysRevB.108.075305*

*Authors:* *S. Pallikkara Chandrasekharan, I. Lucci, D. Gupta, C. Cornet, L. Pedesseau.*

*Laboratories:* *Institut FOTON (fr).*

*Techniques:* *DFT.*

*Materials:* *GaP/Si*

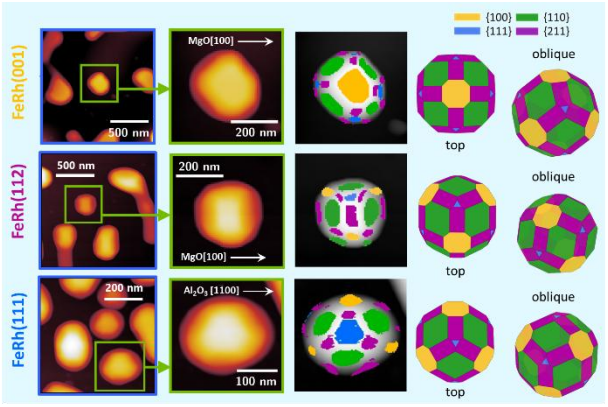
*Abstract*

*Here, we quantitatively determine the impact of III-V/Si interface atomic configuration on the wetting properties of the system. Based on a description at the atomic scale using density functional theory, we first show that it is possible to determine the absolute interface energies in heterogeneous materials systems. A large variety of absolute GaP surface energies and GaP/Si interface energies are then computed, confirming the large stability of charge-compensated III-V/Si interfaces with an energy as low as 23meV/Å2. While stable compensated III-V/Si interfaces are expected to promote complete wetting conditions, it is found that this can be easily counterbalanced by the substrate initial passivation, which favors partial wetting conditions.*

*OPERA Work Group*

*WG1*

## Preserving metamagnetism in self-assembled FeRh nanomagnets




*Reference:* *ACS Appl. Mater. Interfaces 15 (6), 8653-8665 (2023); DOI: 10.1021/acsami.2c20107*

*Authors:* *L. Motyčková, J. A. Arregi, M. Staňo, S. Průša, K. Částková, and V. Uhlíř*

*Laboratories:* *CEITEC Brno University of Technology (Cz)*

*Techniques:* *Magnetron sputtering, XRD, VSM, AFM, MFM, SEM, LEIS*

*Materials:* *FeRh*

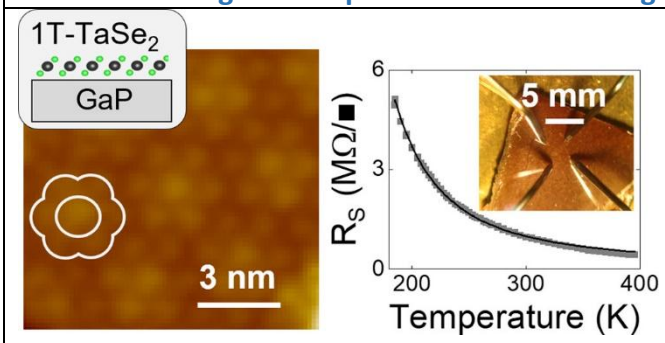
*Abstract*

*Preparing and exploiting phase-change materials in the nanoscale form is an ongoing challenge for advanced material research. A common lasting obstacle is preserving the desired functionality present in the bulk form. Here, we present self-assembly routes of metamagnetic FeRh nanoislands with tunable sizes and shapes. While the phase transition between antiferromagnetic and ferromagnetic orders is largely suppressed in nanoislands formed on oxide substrates via thermodynamic nucleation, we find that nanomagnet arrays formed through solid-state dewetting keep their metamagnetic character. This behavior is strongly dependent on the resulting crystal faceting of the nanoislands, which is characteristic of each assembly route. Comparing the calculated surface energies for each magnetic phase of the nanoislands reveals that metamagnetism can be suppressed or allowed by specific geometrical configurations of the facets. Furthermore, we find that spatial confinement leads to very pronounced supercooling and the absence of phase separation in the nanoislands. Finally, the supported nanomagnets are chemically etched away from the substrates to inspect the phase transition properties of self-standing nanoparticles. We demonstrate that solid-state dewetting is a feasible and scalable way to obtain supported and free-standing FeRh nanomagnets with preserved metamagnetism.*

*OPERA Work Group*

*WG1*

## Large-Area Epitaxial Mott Insulating 1T-$TaSe_2$ Monolayer on $GaP(111)_B$





### Abstract

*Two-dimensional Mott materials have recently been reported in the dichalcogenide family with high potential for Mottronic applications. Nevertheless, their widespread use as a single or few layers is hampered by their limited device integration resulting from their growth on graphene, a metallic substrate. Here, we report on the fabrication of 1T-$TaSe_2$ monolayers grown by molecular beam epitaxy on semiconducting gallium phosphide substrates. At the nanoscale, the charge density wave reconstruction and a moiré pattern resulting from the monolayer interaction with the substrate are observed by scanning tunneling microscopy. The fully open gap unveiled by tunneling spectroscopy, which can be further manipulated by the proximity of a metal tip, is confirmed by transport measurements from micrometric to millimetric scales, demonstrating a robust Mott insulating phase at up to 400 K*



*Reference:* *Nano Lett. 23, 9413 (2023)*

*DOI: 10.1021/acs.nanolett.3c02813*



*Authors:* *H. Koussir, Y. Chernukha, C. Sthioul, E. Haber, N. Peric, L. Biadala, P. Capiod, M. Berthe, I. Lefebvre, X. Wallart, B. Grandidier, and P. Diener*

*Laboratories:* *IEMN (Fr)*

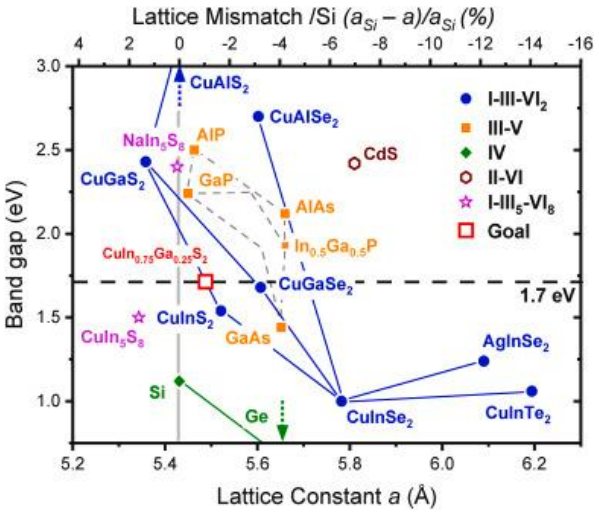

*Techniques:* *STM/STS, MBE, XPS, LEED*

*Materials:* *1T-$TaSe_2$, $GaP(111)_B$*

### OPERA Work Group

*WG1*

## Unveiling the role of copper content in the crystal structure and phase stability of epitaxial Cu(In,Ga)S2 films on GaP/Si(001)





*Reference:* *Mat. Sci. in Semicond. Processing 166, 107685 (2023);*

*DOI: https://doi.org/10.1016/j.mssp.2023.107685*



*Authors:* *E. Bertin, O. Durand, A. Létoublon, C. Cornet, L. Arzel, L. Choubrac, R. Bernard, É. Gautron, S. Harel, M. Jullien, T. Rohel, L. Assmann, N. Barreau*

*Laboratories:* *Institut FOTON (Fr), IMN (Fr)*


*Techniques:* *MBE, co-evaporation, XRD, Raman, EDS.*

*Materials:* *Cu(In,Ga)$S_2$/GaP/Si(001)*

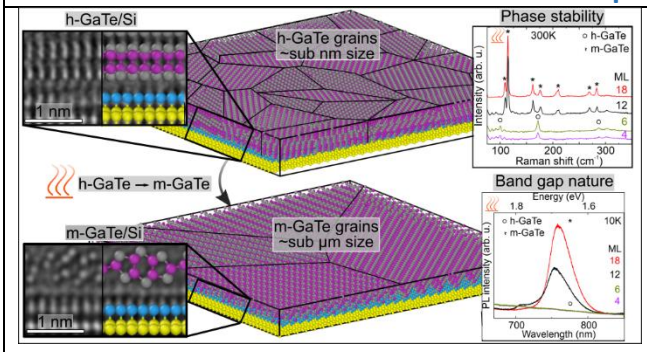

### Abstract

*This study examines the growth condition to obtain a single-phase Cu(In,Ga)$S_2$ (CIGS) chalcopyrite film epitaxially grown by coevaporation on a GaP/Si(001) pseudo-substrate. In particular, we report the structural differences between KCN-etched Cu-rich and Cu-poor CIGS films coevaporated on GaP/Si(001) by 1-stage process. The Cu-poor CIGS film consists of at least three phases; the main crystal is found to be chalcopyrite-ordered, coexisting with In-rich $CuIn_5S_8$, and CuAu-ordered $CuInS_2$, all sharing epitaxial relationships with each other and the GaP/Si(001) pseudo-substrate. On the other hand, the Cu-rich CIGS film is single-phase chalcopyrite and displays sharper X-ray diffraction peaks and a lower density of microtwin defects. The elimination of the secondary CuAu-ordered phase with Cu excess is demonstrated. In both films, the chalcopyrite crystal exclusively grows with its c-axis aligned with the out-of-plane direction of Si[001]. This study confirms prior findings on the thermodynamics of Cu–In-Ga-S and the stability of secondary phases.*


### OPERA Work Group

*WG1*

## Two-dimensional single crystal monoclinic gallium telluride on silicon substrate via transformation of epitaxial hexagonal phase




*Reference:* *npj 2D Materials and Applications 7, 19 (2023); DOI; 10.1038/s41699-023-00390-4*

*Authors:* *E. Zallo, A. Pianetti, A. S. Prikhodko, S. Cecchi, Y. S. Zaytseva, A. Giuliani, M. Kremser, N. I. Borgardt, J. J. Finley, F. Arciprete, M. Palummo, O. Pulci, R. Calarco.*

*Laboratories:* *WSI-Univ. TUM (Ge), Univ. Tor Vergata Rome (It), INFN Rome (It), MIET (Ru), Univ. Milano-Bicocca (It), IMM-CNR Rome (It).*

*Techniques:* *MBE, AFM, TEM, XRD, GID, Raman, RTA, PL, DFT.*

*Materials:* *2D materials, GaTe/Si(111), Sb passivation, phase transformation.*

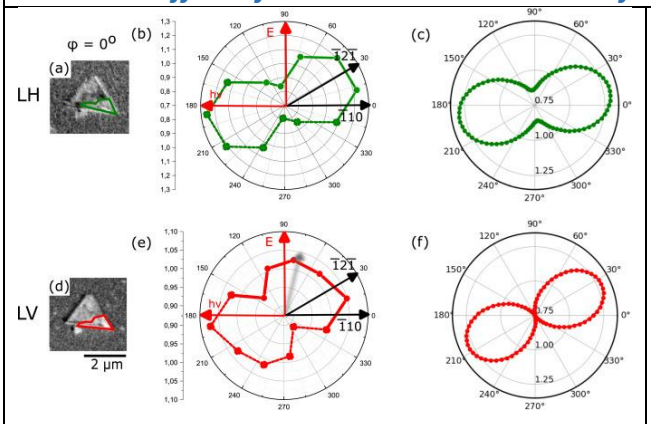
### Abstract

*Van der Waals (vdW) epitaxial growth of large-area and stable two-dimensional (2D) materials of high structural quality on crystalline substrates is crucial for the development of novel device technologies. 2D gallium monochalcogenides with low in-plane symmetry stand out among the layered semiconductor materials family for next-generation optoelectronic and energy conversion applications. Here, we demonstrate the formation of large-area, single crystal and optically active 2D monoclinic gallium telluride (m-GaTe) on silicon substrate via rapid thermal annealing induced phase transformation of vdW epitaxial metastable hexagonal gallium telluride (h-GaTe). Stabilization of multilayer h-GaTe on Si occurs due to the role of the first layer symmetry together with efficient GaTe surface passivation. Moreover, we show that the phase transformation of h-GaTe to m-GaTe is accompanied by the strain relaxation between Si substrate and GaTe. This work opens the way to the fabrication of single-crystal 2D anisotropic semiconductors on standard crystalline wafers that are difficult to be obtained by epitaxial methods.*

### OPERA Work Group

*WG1*

## *Effect of Ni substitution on the antiferromagnetic domains of cobalt oxide*




*Reference:* *Ultramicroscopy 253, 113795 (2023), DOI: 10.1016/j.ultramic.2023.113795*

*Authors:* *A. Mandziak, J. de la Figuera, A. Quesada, A. Berja, J.E. Prieto, C. Granados-Miralles, L. Aballe, M. Foerster, M.A. Niño, P. Nita*

*Laboratories:* *Instituto de Química Física Blas Cabrera (ES), Alba Synchrotron Light Facility (ES), Instituto de Cerámica y Vidrio (ES), Universidad Complutense de Madrid (ES)*

*Techniques:* *MBE*

*Materials:* *Oxides*

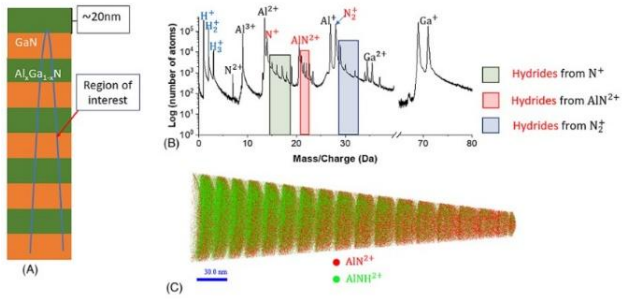
### Abstract

*In this work, We present a spatially resolved X-ray magnetic linear dichroism study of high quality micron-sized mixed nickel-cobalt oxide (NCO) crystals. NiCoO was prepared in-situ by high-temperature oxygen-assisted molecular beam epitaxy on a Ru(0001) single crystal substrate. To check the effect of incorporating Ni into the cobalt oxide films, three different compositions were prepared. The element-specific XMLD measurements reveal strong antiferromagnetic contrast at room temperature and magnetic domains up to one micron in size, reflecting the high structural quality of the NCO islands. By means of vectorial magnetometry, the antiferromagnetic spin axis orientation of the domains was determined with nanometer spatial resolution, and found to depend on the stoichiometry of the prepared crystals.*

### OPERA Work Group

*WG1*

## Field-dependent abundances of hydride molecular ions in atom probe tomography of III-N semiconductors





### Abstract

*We investigate the microscopic behaviour of hydrogen-containing speciesformed on the surface of III-N semiconductor samples by the residual hydro-gen in the analysis chamber in laser-assisted atom probe tomography (APT).We analysed AlGaN/GaN heterostructures containing alternate layers with athickness of about 20 nm. The formation of H-containing species occurs at fieldstrengths between 22 and 26 V/nm and is independent of the analysed samples.The 3D APT reconstruction makes it possible to map the evolution of the surfacebehaviour of these species issued by chemical reactions. The results highlightthe strong dependence of the relative abundances of hydrides on the surfacefield during evaporation. The relative abundances of the hydrides decrease whenthe surface field increases due to the evolution of the tip shape or the differentevaporation behaviour of the different layers.*



*Reference:* *Journal of Microscopy, 1–7 (2023); doi: 10.1111/jmi.13233*



*Authors:* *A. Diagne, L. Gonzalez Garcia, S. Ndiaye, N. Gogneau, M. Vrellou, J. Houard, L. Rigutti.*

*Laboratories:* *Groupe de Physique des Matériaux/CNRS/Rouen Univ. (Fr), C2N/CNRS/Paris-Saclay Univ. (Fr), Karlsruhe Institute of Technology (DE.)*

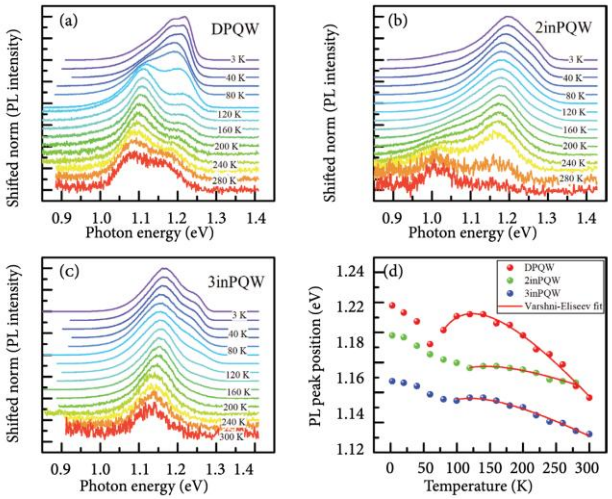

*Techniques:* *PA-MBE, Laser-assisted atom probe tomography*

*Materials:* *AlGaN/GaN heterostructures*

*OPERA Work Group*

*WG1*

## Effects of parabolic barrier design for multiple GaAsBi/AlGaAs quantum well structures





### Abstract

*The results of a comparative study on how the design of multiple quantum structures containing a parabolic barrier profile affects optical properties are presented. All quantum well (QW) structures were grown by molecular beam epitaxy (MBE) on semi-insulating GaAs substrates. The investigated samples consisted of (i) double parabolic quantum wells (type A) or (ii) multiple (two or three) rectangular quantum wells surrounded by parabolic barriers (type B). The optical quality of samples was characterized performing room-temperature (RT-PL) and temperature-dependent photoluminescence (TD-PL) measurements. The investigation revealed benefits of both double parabolic quantum wells and a mixed design (rectangular MQW with parabolic barriers). It was shown that all structures of type A exhibit an intense emission, while the intensity of photoluminescence measured for the samples of type B depends on the number of QWs. The weaker intensity of the PL signal from two QWs inserted between parabolic barriers was explained by a larger point defect density at low temperature grown inner GaAs barriers. The room-temperature PL intensity of the structure with three GaAsBi QWs embedded in one parabolic AlGaAs barrier was the highest one.*



*Reference:* *Lith. J. of Phys., Vol. 63, No. pp. 264-272 (2023); https://doi.org/10.3952/physics.2023.63.4.8*



*Authors:* *M. Jokubauskaitė, G. Petrusevičius, A. Špokas, B. Čechavičius, E. Dudutienė, and R. Butkutė*

*Laboratories:* *Optoelectronics Dept. FTMC (LT)*


*Techniques:* *MBE, PQW, RT-PL, TD-PL*

*Materials:* *GaAsBi and GaAs semiconductors*

*OPERA Work Group*

*WG1*

## BiSb on Flat and Ion-Beam Nano-Patterned InP Substrates


*Reference:* *Physica Status Solidi B (2023) 260: 2300337, DOI: 10.1002/pssb.202300337*

*Authors:* *I. G. Elhoussieny, T. J. Rehaag & G. R. Bell*

*Laboratories:* *University of Warwick, UK*

*Techniques:* *MBE*

*Materials:* *BiSb*

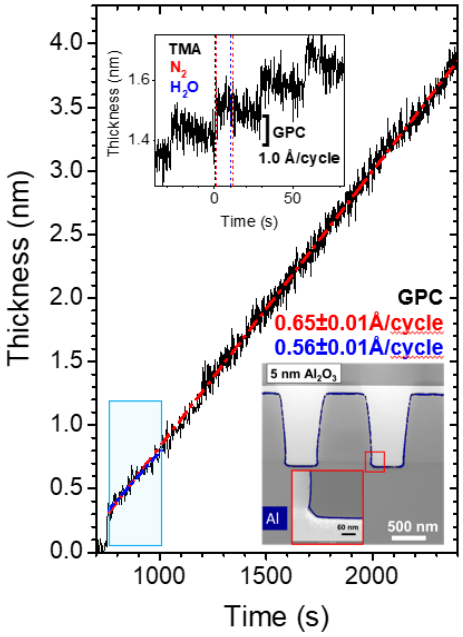
*Abstract*

*BiSb has been grown by MBE on InP substrates which are either flat or nano-patterned using Ar ion beam erosion. Despite identical BiSb growth conditions, the epitaxial orientation of the films is different between the two substrate types: (001) with sixfold in-plane symmetry on flat InP, and (012) with fourfold symmetry on nano-patterned InP. We developed a modified Hall measurement interpretation for non-planar films and extracted a possible contribution to BiSb conductivity from topologically protected surface states.*

*OPERA Work Group*

*WG1*

## Combination of Multiple Operando and In-Situ Characterization Techniques in a Single Cluster System for Atomic Layer Deposition: Unraveling the Early Stages of Growth of Ultrathin $Al_2O_3$ Films on Metallic Ti Substrates.




*Reference:* *Inorganics 11 (2023) 477.*

*DOI: 10.3390/inorganics11120477*

*Authors:* *C. Morales, A. Mahmoodinezhad, R. Tschammer, J. Kosto, C. Alvarado Chavarin, M.A. Schubert, C. Wenger, K. Henkel, J.I. Flege*

*Laboratories:* *BTU-APH (Ger), IHP (Ger)*

*Techniques:* *ALD, XPS, Ellipsometry, QMS, TEM*

*Materials:* *$Al_2O_3$*

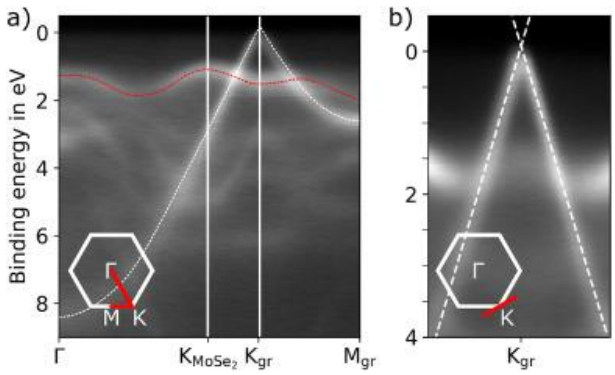
*Abstract*

*This work presents a new ultra-high vacuum cluster tool to perform systematic studies of the early growth stages of atomic layer deposited (ALD) ultrathin films following a surface science approach. By combining operando (spectroscopic ellipsometry and quadrupole mass spectrometry) and in situ (X-ray photoelectron spectroscopy) characterization techniques, the cluster allows us to follow the evolution of substrate, film, and reaction intermediates as a function of the total number of ALD cycles, as well as perform a constant diagnosis and evaluation of the ALD process, detecting possible malfunctions that could affect the growth, reproducibility, and conclusions derived from data analysis. The homemade ALD reactor allows the use of multiple precursors and oxidants and its operation under pump and flow-type modes. To illustrate our experimental approach, we revisit the well-known thermal ALD growth of $Al_2O_3$ using trimethylaluminum and water. We deeply discuss the role of the metallic Ti thin film substrate at room temperature and 200 °C, highlighting the differences between the heterodeposition (<10 cycles) and the homodeposition (>10 cycles) growth regimes at both conditions. This surface science approach will benefit our understanding of the ALD process, paving the way toward more efficient and controllable manufacturing processes.*

*OPERA Work Group*

*WG1*

## Unraveling van der Waals epitaxy: A real-time in-situ study of $MoSe_2$ growth on graphene/Ru(0001)





### Abstract

*In the present work we investigate the growth of monolayer $MoSe_2$ on selenium-intercalated graphene on Ru(0001), a model layered heterostructure combining a transition metal dichalcogenide with graphene, using low energy electron microscopy and micro-diffraction. Real-time observation of $MoSe_2$ on graphene growth reveals the island nucleation dynamics at the nanoscale. Upon annealing, larger islands are formed by sliding and attachment of multiple nanometer-sized $MoSe_2$ flakes. Local micro-spot angle-resolved photoemission spectroscopy reveals the electronic structure of the heterostructure, indicating that no charge transfer occurs within adjacent layers. The observed behavior is attributed to intercalation of Se at the graphene/Ru(0001) interface. The unperturbed nature of the proposed heterostructure therefore renders it as a model system for investigations of graphene supported TMD nanostructures.*



### Reference:

*Ultramicroscopy 250 (2023) 113749*
*DOI: 10.1016/j.ultramic.2023.113749*



### Authors:

*L. Bußß, N. Braud, M. Ewert, M. Jugovac, T. O. Menteş, A. Locatelli, J. Falta, J. I. Flege*


### Laboratories:

*BTU-APH (Ger), Univ. Bremen (Ger), ELETTRA (Italy), MAPEX (Ger)*

### Techniques:

*MBE, LEEM, LEED, ARPES*

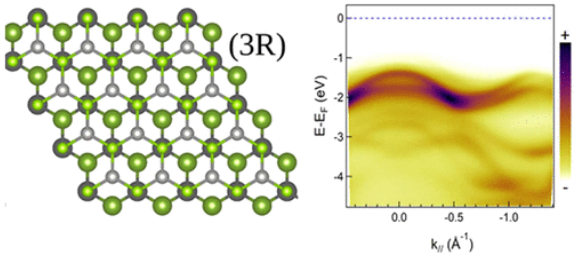
### Materials:

*$MoSe_2$, graphene, Ru(0001)*

### OPERA Work Group

*WG1*

## Quasi van der Waals Epitaxy of Rhombohedral-Stacked Bilayer $WSe_2$ on GaP(111) Heterostructure





### Abstract

The growth of bilayers of two-dimensional (2D) materials on conventional 3D semiconductors results in 2D/3D hybrid heterostructures, which can provide additional advantages over more established 3D semiconductors while retaining some specificities of 2D materials. Understanding and exploiting these phenomena hinge on knowing the electronic properties and the hybridization of these structures. Here, we demonstrate that a rhombohedral-stacked bilayer (AB stacking) can be obtained by molecular beam epitaxy growth of tungsten diselenide ($WSe_2$) on a gallium phosphide (GaP) substrate. We confirm the presence of 3R-stacking of the $WSe_2$ bilayer structure using scanning transmission electron microscopy (STEM) and micro-Raman spectroscopy. Also, we report high-resolution angle-resolved photoemission spectroscopy (ARPES) on our rhombohedral-stacked $WSe_2$ bilayer grown on a $GaP(111)_B$ substrate. Our ARPES measurements confirm the expected valence band structure of $WSe_2$ with the band maximum located at the **Γ** point of the Brillouin zone. The epitaxial growth of $WSe_2/GaP(111)_B$ helps to understand the fundamental properties of these 2D/3D heterostructures, toward their implementation in future devices.



### Reference:

*ACS Nano 17, 21307 (2023)*
*DOI: 10.1021/acsnano.3c05818*



### Authors:

*A. Mahmoudi, M. Bouaziz, N. Chapuis, G. Kremer, J. Chaste, D. Romanin, M. Pala, F. Bertran, P.k Le Fèvre, I. C. Gerber, G. Patriarche, F. Oehler, X. Wallart, and A. Ouerghi*


### Laboratories:

*C2N (Fr), IEMN (Fr), Synchrotron Soleil (Fr), LPCNO (Fr)*

### Techniques:

*ARPES, MBE, STEM, Raman, DFT*

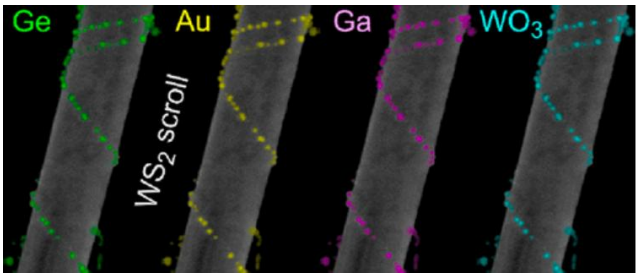
### Materials:

*3R $WSe_2$, $GaP(111)_B$*

### OPERA Work Group

*WG1*

## Chiral Nanoparticle Chains on Inorganic Nanotube Templates




*Reference:* Nano Lett. 23, 6010 (2023); doi: 10.1021/acs.nanolett.3c01213

*Authors:* L. Kachtík, D. Citterberg, K. Bukvišová, L. Kejík, F. Ligmajer, M. Kovařík, T. Musálek, M. Krishnappa, T. Šikola, M. Kolíbal

*Laboratories:* Brno University of Technology (Cz), Holon Institute of Technology (Il)

*Techniques:* MBE, SEM, TEM

*Materials:* $WS_2$, Ge, Au, Ga, $WO_3$

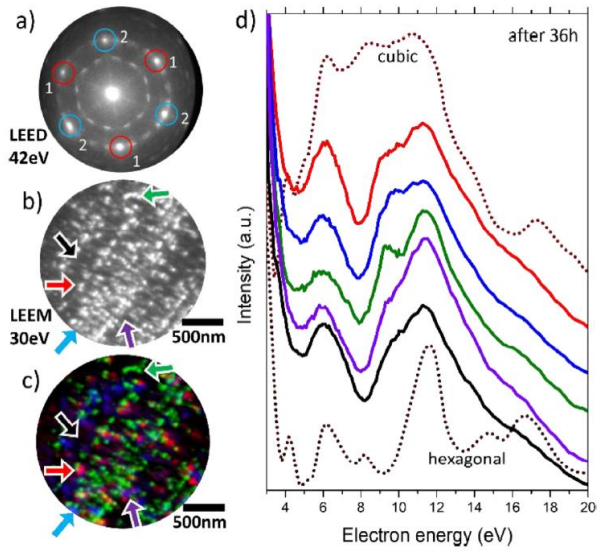

### Abstract

*In this work, we have demonstrated the fabrication of metallic, semiconductor, and oxide nanoparticle chiral assemblies by utilizing scroll-like inorganic nanotube templates. In contrast to the commonly used organic templates, WS2 nanotubes are stable up to 550 °C in a vacuum. Taking advantage of the very high temperature stability of these templates, we have demonstrated the possibility of preparing a wide range of nanoparticle assemblies (metals, oxides, and semiconductors). Scroll-like nanotube templates permit to inscribe chirality to otherwise challenging material systems. The versatility of our approach holds promise for the fabrication of chiroptically active building blocks in emerging areas of chiral nanophotonics, where facile fabrication of such assemblies represents a great challenge. Besides, TMD templates covered with plasmonic nanoparticles could become an ideal playground for studying chiral plasmon–exciton polariton complexes. The proposed fabrication approach thus significantly advances the so-far narrow range of preparation techniques of chiral nanomaterials, allowing for experimental studies of complex chiral systems that have been unavailable up to now.*


*OPERA Work Group*

*WG1*

## Preparation and stability of the hexagonal phase of samarium oxide on Ru(0001)




*Reference:*

*Ultramicroscopy 250 (2023) 113755.*
*DOI: 10.1016/j.ultramic.2023.113755*

*Authors:* E. Pozarowska, L. Pleines, M. Ewert, M. J. Prieto, L. C. Tanase, L. de Souza Caldas, Aarti Tiwari, Thomas Schmidt, J. Falta, E. Krasovskii, C. Morales, J. I. Flege

*Laboratories:* BTU-APH (Ger), Univ. Bremen (Ger), FHI (Ger), IKERBASQUE (Esp), DIPC (Esp), UPV (Esp)

*Techniques:* ALD, XPS, Ellipsometry, QMS, TEM

*Materials:* $Sm_2O_3$, Ru(0001)

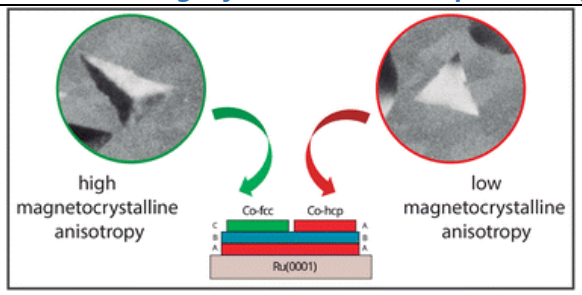

### Abstract

*We have used low-energy electron microscopy (LEEM), micro-illumination low-energy electron diffraction (μLEED) supported by ab initio calculations, and X-ray absorption spectroscopy (XAS) to investigate in-situ and in real-time the structural properties of $Sm_2O_3$ deposits grown on Ru(0001), a rare-earth metal oxide model catalyst. Our results show that samarium oxide grows in a hexagonal A-$Sm_2O_3$ phase on Ru(0001), exhibiting a (0001) oriented-top facet and (113) side facets. Upon annealing, a structural transition from the hexagonal to cubic phase occurs, in which the Sm cations exhibit the +3 oxidation state. The unexpected initial growth in the A-$Sm_2O_3$ hexagonal phase and its gradual transition to a mixture with cubic C-$Sm_2O_3$ showcases the complexity of the system and the critical role of the substrate in the stabilization of the hexagonal phase, which was previously reported only at high pressures and temperatures for bulk samaria. Besides, these results highlight the potential interactions that Sm could have with other catalytic compounds with respect to the here gathered insights on the preparation conditions and the specific compounds with which it interacts.*


*OPERA Work Group*

*WG1*

## Stacking influence on the in-plane magnetic anisotropy in a 2D magnetic system




**Reference:** *Nanoscale 15 (2023) 8313, DOI:10.1039/d3nr00348*

**Authors:** *S. Ruiz-Gómez, L. Pérez, A. Mascaraque, B. Santos, F. El Gabaly, A. K. Schmid and J. de la Figuera*

**Laboratories:** *Instituto de Química Física Blas Cabrera (ES), Universidad Complutense de Madrid (ES), Max-Planck-Institut für Chemische Physik fester Stoffe (DE), Lawrence Berkeley National Laboratory (US)*

**Techniques:** *MBE*

**Materials:** *Metals*

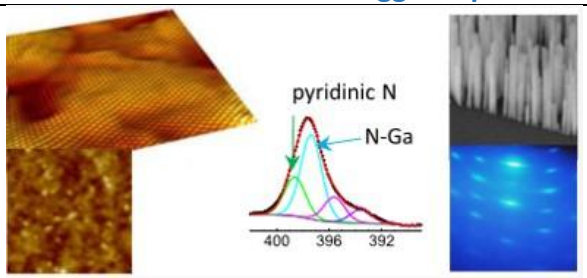
### Abstract

*In this work, The magnetization patterns on three atomic layers thick islands of Co on Ru(0001) are studied by spin-polarized low-energy electron microscopy (SPLEEM). In-plane magnetized micrometer wide triangular Co islands are grown on Ru(0001). They present two different orientations correlated with two different stacking sequences which differ only in the last layer position. The stacking sequence determines the type of magnetization pattern observed: the hcp islands present very wide domain walls, while the fcc islands present domains separated by much narrower domain walls. The former is an extremely low in-plane anisotropy system. We estimate the in-plane magnetic anisotropy of the fcc regions to be 1.96 × 104 J m−3 and of the hcp ones to be 2.5 × 102 J m−3.*

### OPERA Work Group

*WG1*

## What Triggers Epitaxial Growth of GaN on Graphene?




**Reference:** *Cryst. Growth Des. 23, 9, 6517 (2023); doi: 10.1021/acs.cgd.3c00481*

**Authors:** *C. Barbier, L. Largeau, N. Gogneau, L. Travers, C. David, A. Madouri, D. Tamsaout, J-C. Girard, G. Rodary, H. Montigaud, C. Durand, M. Tchernycheva, F. Glas, J-C. Harmand.*

**Laboratories:** *C2N/CNRS/Paris-Saclay Univ. (Fr).*

**Techniques:** *PA-MBE, Raman spectroscopy, AFM, XPS*

**Materials:** *GaN Nanowires on Graphene substrate*

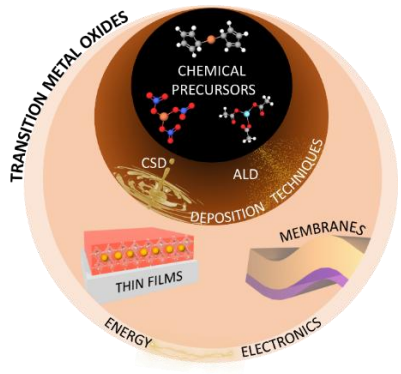
### Abstract

*With the perspective of using two-dimensional materials as growth substrates for semiconductors, we explore the nucleation of GaN nanostructures on graphene. Using plasma-assisted molecular beam epitaxy, we investigate what happens during the long incubation time which precedes the epitaxy of the first GaN islands. After 30 min of nitrogen plasma exposure with no deposition, we find that graphene is modified, and we identify C–N bonds. We measure and model the variation of the incubation time with the growth parameters. These data support the idea that graphene must be modified before GaN nucleation becomes possible. We then test the adhesion at the interface between graphene and the GaN nanostructures. Our studies converge on the conclusion that GaN nanostructures nucleate on graphene from pyridinic N atoms incorporated in the lattice, which are responsible for strong binding between the two materials.*

### OPERA Work Group

*WG1*

## Chemical synthesis of complex oxide thin films and freestanding membranes




*Reference:* Chem. Commun., 2023, 59, 13820-13830; DOI: 10.1039/D3CC03030J

*Authors:* P. Salles, P. Machado, P. Yu and M. Coll

*Laboratories:* ICMAB- CSIC (Spain)

*Techniques:* CSD, ALD

*Materials:* $BiFeO_3$, $La_{0.7}Sr_{0.3}MnO_3$, $CoFe_2O_4$, $Gd_xFe_yO_z$

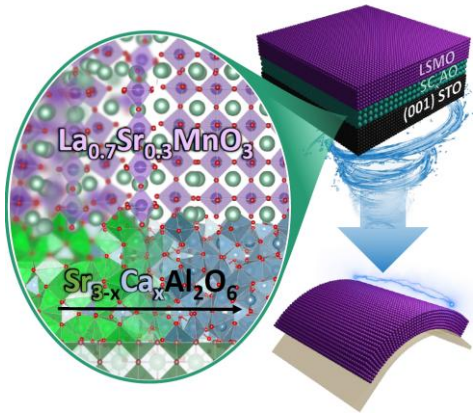
### Abstract

*Oxides offer unique physical and chemical properties that inspire rapid advances in materials chemistry to design and nanoengineer materials compositions and implement them in devices for a myriad of applications. Chemical deposition methods are gaining attention as a versatile approach to develop epitaxial complex oxide thin films and nanostructures by properly selecting compatible chemical precursors and designing an accurate cost-effective thermal treatment. Here, upon describing the basics of chemical solution deposition (CSD) and atomic layer deposition (ALD), some examples of the growth of chemically-deposited functional complex oxide films that can have applications in energy and electronics are discussed. To go one step further, the suitability of these techniques is presented to prepare freestanding complex oxides which can notably broaden their applications. Finally, perspectives on the use of chemical methods to prepare future epitaxial materials are given.*

### OPERA Work Group

WG1

## On the Role of the $Sr_{3-x}Ca_xAl_2O_6$ Sacrificial Layer Composition in Epitaxial $La_{0.7}Sr_{0.3}MnO_3$ Membranes




*Reference:* Adv. Funct. Mater. 2023, 33, 2304059; https://doi.org/10.1002/adfm.202304059

*Authors:* P. Salles, R. Guzman, A. Barrera, M. Ramis, JM. Caicedo, A. Palau, W. Zhou, M. Coll

*Laboratories:* ICMAB- CSIC (Spain), UCAS (China), ICN2 (Spain)

*Techniques:* CSD, PLD, XRD, RHEED, STEM, PPMS electrical conductivity.

*Materials:* $Sr_{3-x}Ca_xAl_2O_6$, $La_{0.7}Sr_{0.3}MnO_3$,

### Abstract

*The possibility to fabricate freestanding single crystal complex oxide films has raised enormous interest to be integrated in next-generation electronic devices envisaging distinct and novel properties that can deliver unprecedented performance improvement compared to traditional semiconductors. The use of the water-soluble $Sr_3Al_2O_6$ (SAO) sacrificial layer to detach the complex oxide film from the growth substrate has significantly expanded the complex oxide perovskite membranes library. Nonetheless, the extreme water sensitivity of SAO hinders its manipulation in ambient conditions and restricts the deposition approaches to those using high vacuum.*

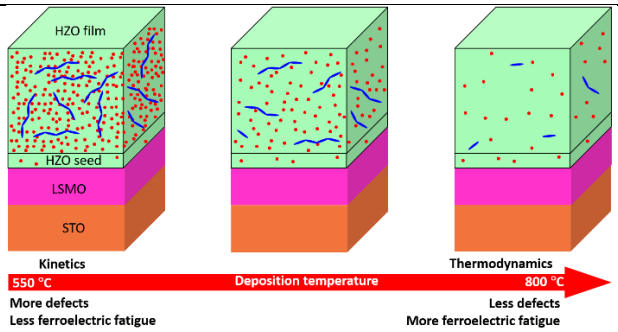
*This study presents a pioneering study on the role of Ca-substitution in solution processed SAO ($Sr_{3-x}Ca_xAl_2O_6$ with $x \leqslant 3$) identifying a noticeable improvement on surface film crystallinity preserving a smooth surface morphology while favoring the manipulation in a less-restricted ambient conditions. Then, the study focuses on the effect of the sacrificial composition on the subsequent ex situ deposition of $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) by pulsed laser deposition, to obtain epitaxial films with a variable degree of strain. Finally, epitaxial and strain-free LSMO membranes with metal-insulator transition at 290 K are delivered. This study offers a hybrid and versatile approach to prepare and easily manipulate crystalline perovskite oxide membranes by facilitating ex situ growth on SAO-based sacrificial layer.*

### OPERA Work Group

WG1

# II- From fundamental research to applications (WG1&WG2)

## Ferroelectric $Hf_{0.5}Zr_{0.5}O_2$ films with improved endurance by low temperature epitaxial growth on seed layers




*Reference:* *Nanoscale 2023, 15, 5293; DOI: 10.1039/D2NR05935E*

*Authors:* *T. Song, R. Bachelet, G. Saint-Girons, I. Fina, F. Sánchez*

*Laboratories:* *Institut de Ciència de Materials de Barcelona (ICMAB-CSIC) (Es), Institut des Nanotechnologies de Lyon - INL (Fr)*

*Techniques:* *PLD, MBE, ferroelectric loops and reliability, AFM, XRD*

*Materials:* *doped $HfO_2$ on $La_{0.67}Sr_{0.33}MnO_3/SrTiO_3(001)$ and Si(001)*

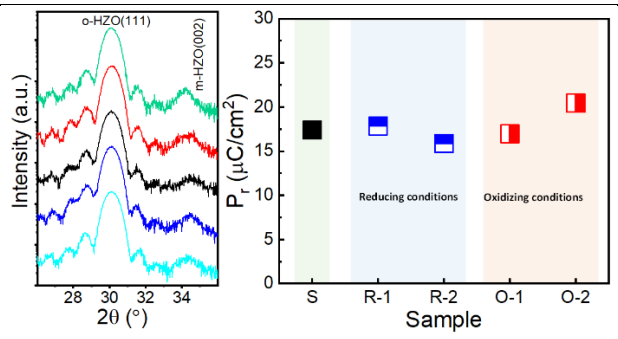

### Abstract

*The crystallization temperature is a critical parameter in the stabilization of the metastable ferroelectric phase of $HfO_2$. The optimal crystallization temperature used for polycrystalline films is too low to grow epitaxial films. We have developed a new growth strategy, based on the use of an ultrathin seed layer, to obtain high-quality epitaxial films of orthorhombic $Hf_{0.5}Zr_{0.5}O_2$ at lower temperature. The threshold temperature for epitaxy is reduced from about 750 ℃ to about 550 ℃ by using a seed layer. Epitaxial films deposited at low temperature exhibit highly enhanced endurance, and films grown at 550 - 600 ℃ have high polarization, no wake-up effect, and greatly reduced fatigue and improved endurance in comparison with the films deposited at high temperature without a seed layer. We propose that the endurance enhancement is due to a positive effect of the defects, which limit the propagation of pinned ferroelectric domains.*


*OPERA Work Group*

*WG1 & WG2*

## Ferroelectric $Hf_{0.5}Zr_{0.5}O_2$ films with improved endurance by low temperature epitaxial growth on seed layers




*Reference:* *ACS Applied Electronic Materials 2023, 5, 6142; DOI: 10.1021/acsaelm.3c01085*

*Authors:* *X. Lyu, T. Song, A. Quintana, I. Fina, F. Sánchez*

*Laboratories:* *Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), (Es)*

*Techniques:* *PLD, ferroelectric loops and reliability, AFM, XRD*

*Materials:* *doped $HfO_2$ on $La_{0.67}Sr_{0.33}MnO_3/SrTiO_3(001)$*

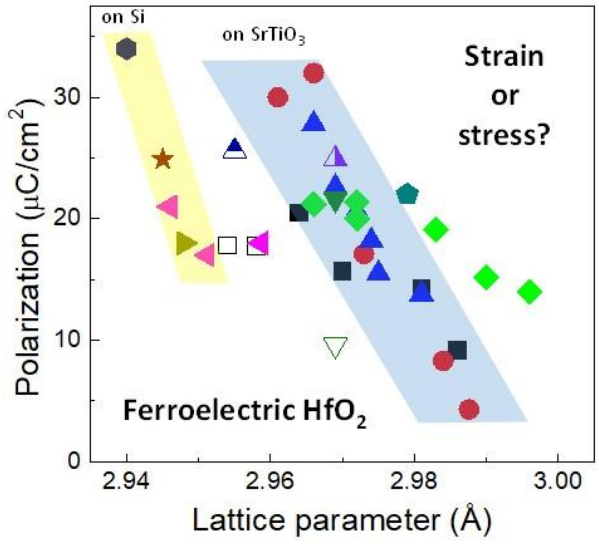

### Abstract

*Cooling conditions are critical in the crystallization of polycrystalline films of ferroelectric $HfO_2$ because the energy of the $HfO_2$ polymorphs is very sensitive to oxygen vacancies and because of the role of kinetics on the stabilization of the metastable orthorhombic phase. Here we investigate the relevance of cooling conditions in pulsed laser deposition of epitaxial $Hf_{0.5}Zr_{0.5}O_2$ films. The orthorhombic phase crystallized in epitaxial $Hf_{0.5}Zr_{0.5}O_2$ films does not change when highly reducing or oxidizing cooling conditions are used. The films exhibit similar ferroelectric properties, including polarization value, absence of wake up effect, comparable fatigue and high retention. These results demonstrate that the phases formed in epitaxial films are highly stable and much less sensitive to cooling conditions than polycrystalline films.*


*OPERA Work Group*

*WG1 & WG2*

## Disentangling stress and strain effects in ferroelectric $HfO_2$





### Abstract

*Ferroelectric $HfO_2$ films are usually polycrystalline and contain a mixture of polar and nonpolar phases. This challenges the understanding and control of polar phase stabilization and ferroelectric properties. Several factors such as dopants, oxygen vacancies, or stress, among others, have been investigated and shown to have a crucial role on optimizing the ferroelectric response. Stress generated during deposition or annealing of thin films is a main factor determining the formed crystal phases and influences the lattice strain of the polar orthorhombic phase. It is difficult to discriminate between stress and strain effects on polycrystalline ferroelectric $HfO_2$ films, and the direct impact of orthorhombic lattice strain on ferroelectric polarization has yet to be determined experimentally. Here, we analyze the crystalline phases and lattice strain of several series of doped $HfO_2$ epitaxial films. We conclude that stress has a critical influence on metastable orthorhombic phase stabilization and ferroelectric polarization. On the contrary, the lattice deformation effects are much smaller than those caused by variations in the orthorhombic phase content. The experimental results are confirmed by density functional theory calculations on $HfO_2$ and $Hf_{0.5}Zr_{0.5}O_2$ ferroelectric phases.*



*Reference:* *Applied Physics Reviews 2023, 10, 041415; DOI: 10.1063/5.0172259*



*Authors:* *T. Song, V. Lenzi, J.P.B. Silva, L. Marques, I. Fina, F. Sánchez*

*Laboratories:* *Institut de Ciència de Materials de Barcelona (ICMAB-CSIC) (Es), University of Aveiro (Pt), University of Minho (Pt)*

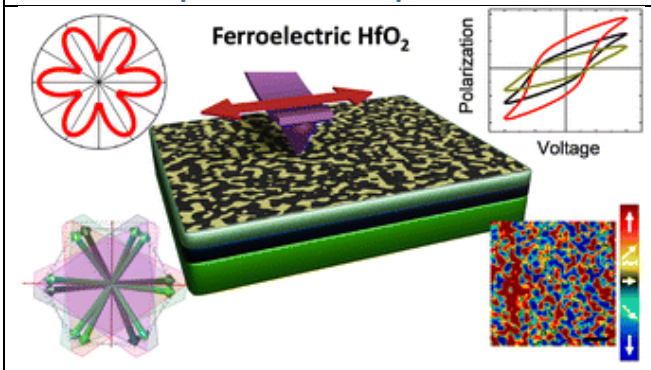

*Techniques:* *PLD, ferroelectric loops, AFM, XRD, DFT*

*Materials:* *doped $HfO_2$ on $La_{0.67}Sr_{0.33}MnO_3/SrTiO_3(001)$*

*OPERA Work Group*

*WG1 & WG2*

## Vector piezoelectric response and ferroelectric domain formation in $Hf_{0.5}Zr_{0.5}O_2$ films





### Abstract

*The piezoelectric response in polycrystalline films of doped ferroelectric $HfO_2$ has been explored so far; however, the lack of texture in most of the studied films prevents its full understanding. By selecting the appropriate substrate orientation, the ferroelectric orthorhombic phase ratio and crystallographic orientation can be modified in epitaxial films. We exploit this possibility to get further insight into the ferroelectric hafnium oxide piezoelectric response. While characterizing in-plane and out-of-plane piezoelectric responses, it is observed that their magnitude is mainly ruled by the presence of the orthorhombic phase and the polar axis of the polarization along the probing direction. It is also found for the as-grown state that along the out-of-plane direction a single ferroelectric domain is formed, and instead the in-plane response reveals a rich domain structure with a domain size of ≈10–30 nm. By characterizing the in-plane piezoelectric response, it is observed that it is anisotropic if the specific orientation, (110), of the $SrTiO_3$ substrate is used. We propose that an out-of-plane single domain is formed due to the presence of an imprint electric field, whereas in-plane domains are formed by non-purely electrostatic interactions as revealed by their relatively large size. Besides, the small but sizeable in-plane anisotropic response is found to result from the in-plane crystallographic configuration, ultimately determined by the selected substrate.*



*Reference:* *Journal of Materials Chemistry C 2023, 11, 7219; DOI: 10.1039/D3TC01145C*



*Authors:* *H. Tan, T. Song, N. Dix, F. Sánchez, I. Fina*

*Laboratories:* *Institut de Ciència de Materials de Barcelona (ICMAB-CSIC) (Es)*


*Techniques:* *PLD, ferroelectric loops, PFM*

*Materials:* *doped $HfO_2$ on $La_{0.67}Sr_{0.33}MnO_3/SrTiO_3(001-110-111)$*

*OPERA Work Group*

*WG1 & WG2*

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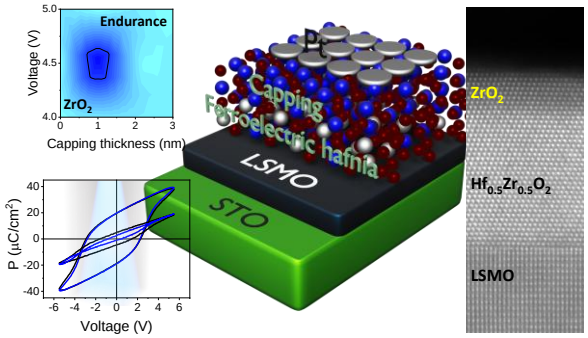
## Improved Polarization-Retention-Endurance in $Hf_{0.5}Zr_{0.5}O_2$ Films by $ZrO_2$ Capping via Electrostatic Effects





### Abstract

*Ferroelectric hafnia is one of the most promising materials for next generation of non-volatile memory devices. Several strategies have demonstrated to be of interest to improve its functional properties. Interface engineering, realized by the introduction of additional layer in the capacitor structure, is demonstrated as a promising strategy. However, interface layers can have multiple implications, such as changes in the chemistry of the interfaces and an increase of depolarization field, whose effects are difficult to discriminate. The role of $HfO_2$ and $ZrO_2$ capping is explored on polarization, retention, endurance, and leakage properties of $Hf_{0.5}Zr_{0.5}O_2$ epitaxial films. In $HfO_2$ capped films, lower polarization is observed, and endurance and retention are also comparably worse than in $ZrO_2$ capped films. Complementary under illumination ferroelectric characterization and capacitance measurements indicate a reduction of defects and interface capacitance contribution in $ZrO_2$ capped films. For both cappings, the interfaces with the $Hf_{0.5}Zr_{0.5}O_2$ layer are shown to be compositionally sharp and the phase of $Hf_{0.5}Zr_{0.5}O_2$ (HZO) grains is replicated on the capping layer, indicating that electrostatic effects prevail and that the use of interface layers with high permittivity, here $ZrO_2$, is crucial to favor good functional properties.*



*Reference:* *Advanced Electronic Materials 2023; DOI: 10.1002/aelm.202300509*



*Authors:* *T. Song, P. Koutsogiannis, C. Magén, J.A. Pardo, F. Sánchez, I. Fina*

*Laboratories:* *Institut de Ciència de Materials de Barcelona (ICMAB-CSIC) (Es), Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza (ES)*

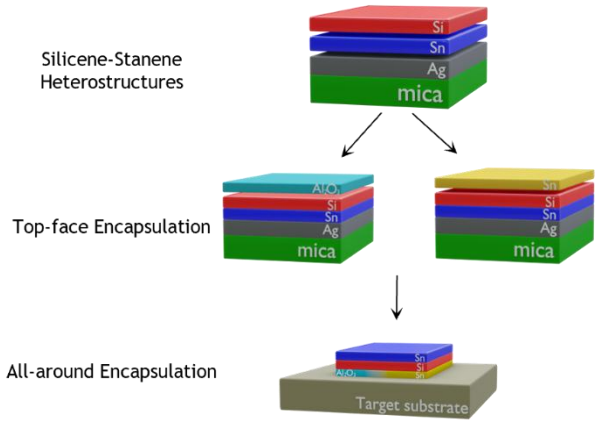

*Techniques:* *PLD, ferroelectric loops, endurance, retention, TEM*

*Materials:* *doped $HfO_2$ on $La_{0.67}Sr_{0.33}MnO_3/SrTiO_3(001)$*

*OPERA Work Group*

*WG1 & WG2*

## All-Around Encapsulation of Silicene





### Abstract

*Silicene or the two-dimensional (2D) graphene-like silicon allotrope has recently emerged as a promising candidate for various applications in nanotechnology. However, concerns on the silicene stability still persist to date and need to be addressed aiming at the fabrication of competing and durable silicene-based devices. Here, we present an all-around encapsulation methodology beyond the current state-of-the-art silicene configuration, namely silicene sandwiched in between a capping layer (e.g., $Al_2O_3$) and the supporting substrate (e.g., Ag). In this framework, the insertion of one or two sacrificial 2D Sn layers enables the realization of different atomically thin encapsulation schemes, preserving the pristine properties of silicene while decoupling it from the growth template. On one hand, the epitaxy of a 2D Sn layer before silicene allows for the removal of the Ag substrate with no effect on silicene which in turn can be easily gated, for example, with an oxide layer on its top face. On the other hand, a full 2D encapsulation scheme, where top and bottom faces of silicene are protected by 2D Sn layers, gives rise to an atomically thin and $cm^2$-scaled membrane preventing degradation of silicene for months. Both schemes thus constitute an advancement for the silicene stability and encapsulation in ambient conditions, paving the way to further exploitation in flexible electronics and photonics.*



*Reference:* *Nanoscale Horizons, 8, 1428 (2023); DOI: 10.1039/D3NH00309D*



*Authors:* *D. S. Dhungana, C. Massetti, C. Martella, C. Grazianetti, A. Molle*

*Laboratories:* *CNR-IMM (It)*

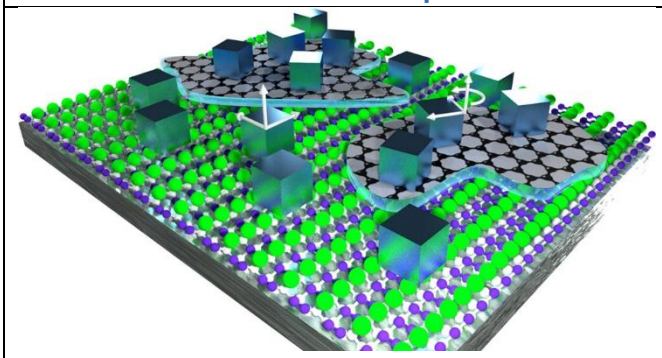

*Techniques:* *MBE, Raman Spectroscopy, XPS*

*Materials:* *Silicene, Stanene*

*OPERA Work Group*

*WG1 & WG2*

## Tiling the Silicon for Added Functionality: PLD Growth of Highly Crystalline STO and PZT on Graphene Oxide-Buffered Silicon Surface



*Reference:* ACS Appl. Mater. Interfaces **15** (2023) 6058−6068; doi: https://doi.org/10.1021/acsami.2c17351

*Authors:* Zoran Jovanović, Urška Trstenjak, Hsin-Chia Ho, Olena Butsyk, Binbin Chen, Elena Tchernychova, Fedir Borodavka, Gertjan Koster, Jiří Hlinka, and Matjaž Spreitzer

*Laboratories:* Jožef Stefan Institute (Sl), University of Belgrade (Rs), Czech Academy of Sciences (Cz), University of Twente (Nl), East China Normal University (Cn), National Institute of Chemistry (Sl)

*Techniques:* PLD, RHEED, SEM, TEM, XRD, AFM, EDS, electrical characterization, etc.

*Materials:* silicon, rGO, STO, PZT

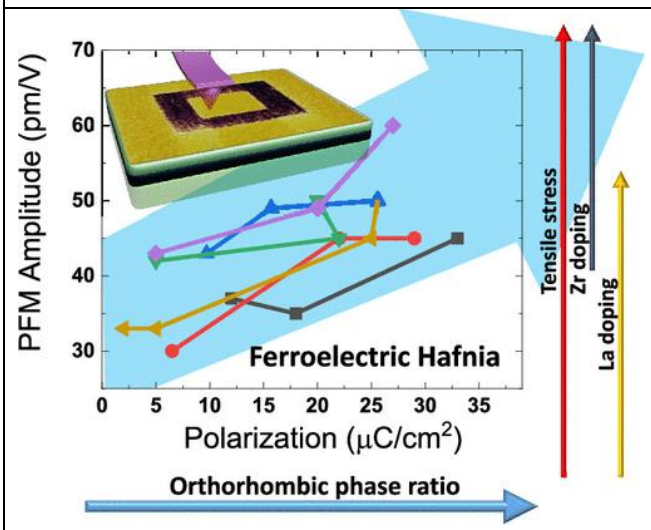
*Abstract*

*The application of two-dimensional (2D) materials has alleviated a number of challenges of traditional epitaxy and pushed forward the integration of dissimilar materials. Besides acting as a seed layer for van der Waals epitaxy, the 2D materials – being atom(s) thick – have also enabled wetting transparency in which the potential field of the substrate, although partially screened, is still capable of imposing epitaxial overgrowth. One of the crucial steps in this technology is the preservation of the quality of 2D materials during and after their transfer to a substrate of interest. In the present study, we show that by honing the achievements of traditional epitaxy and wet chemistry a hybrid approach can be devised that offers a unique perspective for the integration of functional oxides with a silicon platform. It is based on SrO-assisted deoxidation and controllable coverage of silicon surface with a layer(s) of spin-coated graphene oxide, thus simultaneously allowing both direct and van der Waals epitaxy of SrTiO3 (STO). We were able to grow a high-quality STO pseudo-substrate suitable for further overgrowth of functional oxides, such as PbZr1–xTixO3 (PZT). Given that the quality of the films grown on a reduced graphene oxide-buffer layer was almost identical to that obtained on SiC-derived graphene, we believe that this approach may provide new routes for direct and "remote" epitaxy or layer-transfer techniques of dissimilar material systems.*

*OPERA Work Group*

*WG1 & WG2*

## Effects of Doping, Stress, and Thickness on the Piezoelectric Response and Its Relation with Polarization in Ferroelectric $HfO_2$




*Reference:* ACS Appl. Electron. Mater. 2023, ; DOI: 10.1021/acsaelm.3c01154

*Authors:* H Tan, S Estandía, F Sánchez, I Fina

*Laboratories:* Institut de Ciència de Materials de Barcelona (ICMAB-CSIC) (Es)

*Techniques:* PLD, PFM, TEM

*Materials:* doped $HfO_2$

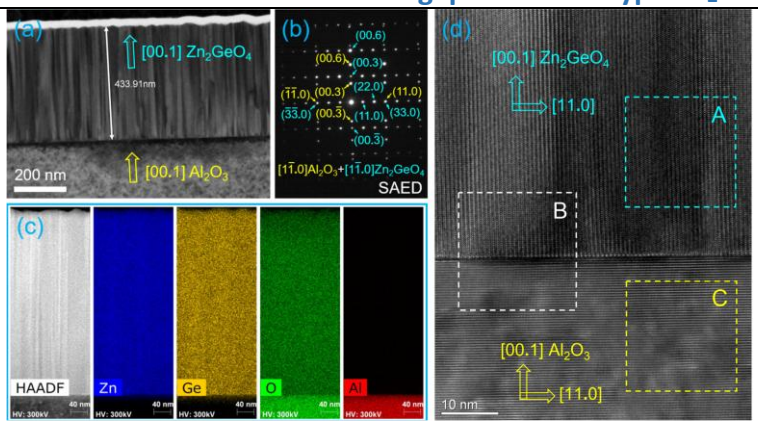
*Abstract*

*The piezoelectric response in hafnia is of interest because it is a CMOS-compatible material. It is known that polarization depends on the stabilization of the orthorhombic phase, which depends on several parameters, such as doping, stress, and thickness. Here, the piezoelectric response in epitaxial doped $HfO_2$ films characterized by piezoelectric force microscopy, is investigated considering this multifactorial dependence. The impact of different levels of La and Zr doping, variations of stress effects controlled by substrate selection, and thickness effects on piezoresponse is analyzed. It is found that the piezoelectric response is mainly correlated with the polarization, i.e., it is primarily determined by the amount of the orthorhombic phase. Interestingly, Zr doping of hafnia is observed to result in a larger piezoresponse than La doping for films showing similar polarization. The piezoresponse is found to be the greatest for the pure $ZrO_2$ film; however, the actual ferroelectric response is not observed by piezoelectric force microscopy, indicating an exception to the general tendency. It is concluded that in the case of samples showing larger amounts of the orthorhombic phase, extrinsic effects due to the tip radii effect can influence the evaluation of the amplitude of the piezoresponse.*

*OPERA Work Group*

*WG1 & WG2*

## Ultrawide bandgap willemite-type $Zn_2GeO_4$ epitaxial thin films




*Reference:* *Appl. Phys. Lett. 122, 031601 (2023); DOI: 10.1063/5.0130946*

*Authors:* *S. Luo, L. Trefflich, S. Selle, R. Hildebrandt, E. Krüger, S. Lange, J. Yu, C. Sturm, M. Lorenz, H. von Wenckstern, C. Hagendorf, T. Höche, and M. Grundmann*

*Laboratories:* *Universität Leipzig (De), Fraunhofer Institute for Microstructure of Materials and Systems Halle (De), Fraunhofer Center for Silicon Photovoltaics CSP Halle (De)*

*Techniques:* *PLD, XRD, AFM, STEM-EDX, HR-TEM, XPS, PL, UV-VIS, DFT*

*Materials:* *$Zn_2GeO_4$*

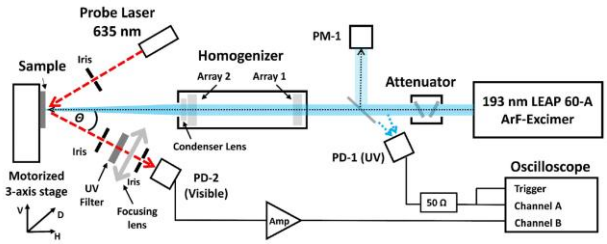
### Abstract

*The Willemite-type $Zn_2GeO_4$ is a promising ultrawide bandgap semiconductor material. Here, we report the heteroepitaxial growth of (00.1)-oriented $Zn_2GeO_4$ thin films on c-plane sapphire substrates using pulsed laser deposition. A 450 nm thick epitaxial film with a surface roughness of 2.5 nm deposited under 0.1 mbar oxygen partial pressure exhibits a full width at half maximum (FWHM) of rocking curve of (00.6) reflex of 0.35°. The direct bandgap is evaluated to be 4.9 ± 0.1 eV. The valence band maximum is determined to be 3.7 ± 0.1 eV below the Fermi level. From DFT band structure calculation, it is suggested that the O 2p orbital and Zn 3d orbital dominantly contribute to the valence band of $Zn_2GeO_4$. This work advances the fundamental study on willemite-type $Zn_2GeO_4$ epitaxial thin films for potential device application.*

### OPERA Work Group

*WG 1 & WG2*

## Pulsed 193 nm Excimer laser processing of 4H–SiC (0001) wafers with radiant exposure dependent in situ reflectivity studies for process optimization




*Reference:* *Mater. Sci. Semicond. Process. 168 (2023) 107839 https://doi.org/10.1016/j.mssp.2023.107839*

*Authors:* *A.P. Menduiña, A.F. Doval, R. Delmdahl, E. Martin, K. Kant, J.L. Alonso-Gómez, S. Chiussi*

*Laboratories:* *FA3-CINTECX ,CINBIO, IFCA, Univ.Vigo (E), Coherent LaserSytems (D).*

*Techniques:* *ELA, ELC, UV-Laser ablation, TRR, Raman, Numerical simulation.*

*Materials:* *SiC, Group-IV semiconductors, graphene*

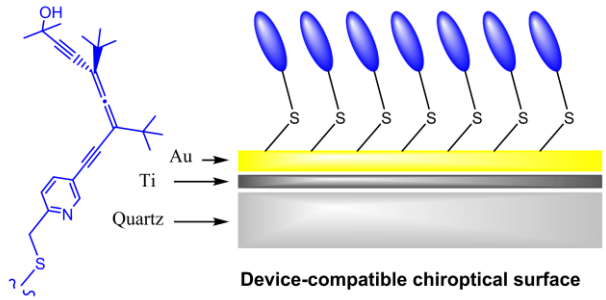
### Abstract

*Excimer lasers are efficient tools to process group-IV semiconductors for advanced microelectronic and photonic devices through crystallization, annealing, or strain engineering. This paper presents a first study of different 193 nm laser processes using a new generation of industrial High power Excimer lasers, applied to SiC wafer surfaces. As a result of this evaluation, specific experimental windows for these processes can now be studied, aiming the creation, and annealing of vacancies for quantum electronics and spintronics, the melting of metals with shallow SiC surface regions to improve electrical contacts, and the production of specific Graphene rich surface patterns on SiC for new device concepts. To develop such laser assisted processes and optimize process parameters, a numerical simulation of the laser/material interaction is essential. This study therefore evaluates the temporal profile of a new high-power 193 nm Excimer laser, and presents the results of in-situ Time Resolved Reflectivity (TRR) measurements obtained when irradiating 4H–SiC(0001) wafers with radiant exposures ranging from 0,1 J/cm² to 3,0 J/cm². The temporal pulse profile is determined, fitted and applied in a 1-D numerical simulation of the temperature gradients for Si(100) as reference sample, to validate the experimental findings. Radiant exposure thresholds at around 1,4 J/cm2 to locally produce molten surfaces and 1,8 J/cm2 to ablate and create carbon-rich regions with graphene, are determined in-situ and confirmed by Raman spectroscopy.*

### OPERA Work Group

*WG1, WG2*

## Development of robust chiroptical systems through spirobifluorenes



Device-compatible chiroptical surface

*Reference:* *Chirality. 2023; 1-7. https://doi.org/10.1002/chir.23624*

*Authors:* *J. Portela-Pino, M.Talavera, S.Chiussi, S.Bolaño, A. Peña-Gallego, J. Lorenzo Alonso-Gómez*

*Laboratories:* *FA3-CINTECX, Univ.Vigo (E).*

*Techniques:* *PVD, Dip coating.*

*Materials:* *Chiroptical molecules, Devise compatible Upstanding architectures (UCAs)*


### Abstract

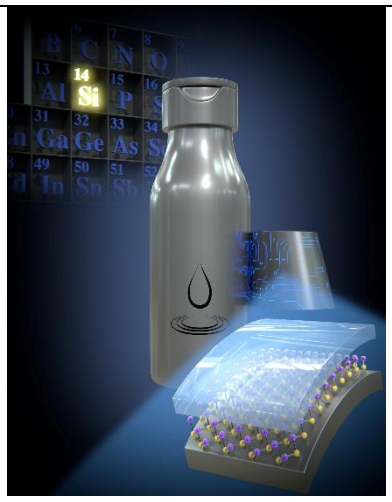
*Chiroptical responses are valuable for the structural determination of dissymmetric molecules. However, the development of everyday applications based on chiroptical systems is yet to come. We have been earlier using axially chiral allenes for the construction of linear, cyclic, and cage-shaped molecules that present remarkable chiroptical responses. Additionally, we have developed chiral surfaces through upstanding chiral architectures. A precise alignment of these upstanding chiral architectures (UCA's) on heteroepitaxial devise structures could lead to the development of new devices, such as spin filters, optical switches and sensors for spintronic, photonic and biomedical applications. Since the challenge is to obtain robust chiroptical materials, we have been studying spirobifluorenes (SBFs), a well-established building block in optoelectronic applications.*

*After theoretical and experimental demonstration, the suitability of chiral SBFs for the development of robust chiroptical systems was certified by the construction all-carbon double helices, flexible shape-persistent macrocycles, chiral frameworks for surface functionalization, and structures featuring helical or spiroconjugated molecular orbitals. Here, we give an overview of our contribution to these matters.*


### OPERA Work Group

*WG1, WG2*

## Epitaxial Synthesis of Silicene and Transfer on Flexible Substrates for Bendable Silicene Membranes Fabrication




*Reference:* *Adv. Mater. 35, 2211419 (2023); DOI: 10.1002/adma.202211419*

*Authors:* *C. Martella, C. Massetti, D. S. Dhungana, E. Bonera, C. Grazianetti, A. Molle*

*Laboratories:* *CNR-IMM (It), Univ. Milano-Bicocca (It)*

*Techniques:* *MBE, Raman Spectroscopy, electrical measurements*

*Materials:* *Silicene*


### Abstract

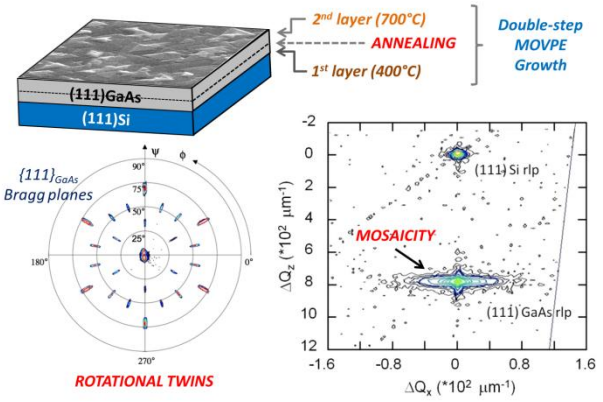
*Due to their superior mechanical properties, 2D materials have gained interest as active layers in flexible devices co-integrating electronic, photonic, and straintronic functions altogether. To this end, 2D bendable membranes compatible with the technological process standards and endowed with large-scale uniformity are highly desired. Here, it is reported on the realization of bendable membranes based on silicene layers (the 2D form of silicon) by means of a process in which the layers are fully detached from the native substrate and transferred onto arbitrary flexible substrates. The application of macroscopic mechanical deformations induces a strain-responsive behavior in the Raman spectrum of silicene. It is also shown that the membranes under elastic tension relaxation are prone to form microscale wrinkles displaying a local generation of strain in the silicene layer consistent with that observed under macroscopic mechanical deformation. Optothermal Raman spectroscopy measurements reveal a curvature-dependent heat dispersion in silicene wrinkles. Finally, as compelling evidence of the technological potential of the silicene membranes, it is demonstrated that they can be readily introduced into a lithographic process flow resulting in the definition of flexible device-ready architectures, a piezoresistor, and thus paving the way to a viable advance in a fully silicon-compatible technology framework.*


### OPERA Work Group

*WG1 & WG2*

# III- Applications- and Industry-oriented material developments (WG2&3)

## GaAs hetero-epitaxial layers grown by MOVPE on exactly-oriented and off-cut (111)Si: Lattice tilt, mosaicity and defects content





### Abstract

*Integration of III-V devices with Si-photonics and fabrication of monolithic III-V/Si tandem solar cells require the heteroepitaxy of III-V compounds on Si. We report on the lattice tilt, mosaicity and defects content of relaxed GaAs grown by MOVPE on exactly-oriented and 4°-offcut (111)Si. Thin GaAs single-layers grown at 400 °C and annealed at 700 °C show ~3×10$^{8}$ cm$^{-2}$ density of surface pinholes. Double-layer samples were obtained by GaAs overgrowth at 700 °C. GaAs epilayers are tilted by (0.05–0.14)° with respect to Si. Rotational twins were observed in X-ray diffraction (XRD) pole figures: the most abundant ones originate from 60°-rotation of GaAs around the [$\bar{1}\bar{1}\bar{1}$] growth direction and are identified as micro-twins along the GaAs/Si hetero-interface. Twins obtained by rotations around the [$\bar{1}\bar{1}\bar{1}$], [$1\bar{1}\bar{1}$], and [$\bar{1}1\bar{1}$] directions or by combined rotations around the growth direction and one of the former, were also observed. The GaAs mosaicity and block size were studied through high-resolution XRD intensity mapping: for single-layer samples crystal blocks are ascribed to 3–5 nm thin microtwins, whose size does not change upon annealing. In double-layer samples thicker (32–35 nm) micro-twins occur. GaAs samples grown on offcut (111)Si show less rotational twins but a reduced mosaic block size with respect to exactly-oriented Si.*



**Reference:** *Applied Surface Science 634 (2023) 157627; DOI: 10.1016/j.apsusc.2023.157627*

**Authors:** *N. Lovergine, I. Miccoli, L. Tapfer , P. Prete*

**Laboratories:** *IMM-CNR (It), Univ. Salento (It)*

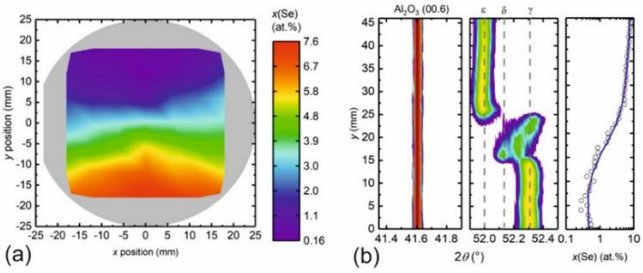
**Techniques:** *MOCVD, XRD, Photoreflectance, FESEM.*

**Materials:** *GaAs, silicon*


**OPERA Work Group**

*WG2*

## Flexible Hardware Concept of Pulsed Laser Deposition for Large Areas and Combinatorial Composition Spreads





### Abstract

*Pulsed Laser Deposition (PLD) is one of the most flexible physical growth techniques for thin films of functional materials at the research and demonstrator level. We describe a relatively simple and reliable concept of the PLD hardware which allows both deposition on large-areas up to 4-inch diameter and of tailored lateral and vertical composition spreads without time-consuming hardware changes. The particular growth mode is selected by the computer-controlled movement of target and substrate together with a suitable target phase composition.*
*The Figure shows: (a) the lateral distribution of the chemical composition on a 2-inch diameter selenium-doped CuI film on c-plane sapphire, grown by a combinatorial PLD technique using a segmented target, and (b) the XRD line scan along the selenium gradient (y-scale) aligned vertically in (a) with a phase separation of CuI:Se around 1 at% Se.*



**Reference:** *Rev. Sci. Instrum. 94, 083905 (2023); DOI: https://doi.org/10.1063/5.0142085*

**Authors:** *M. Lorenz, H. Hochmuth, H. von Wenckstern, M. Grundmann*

**Laboratories:** *Universität Leipzig (De)*

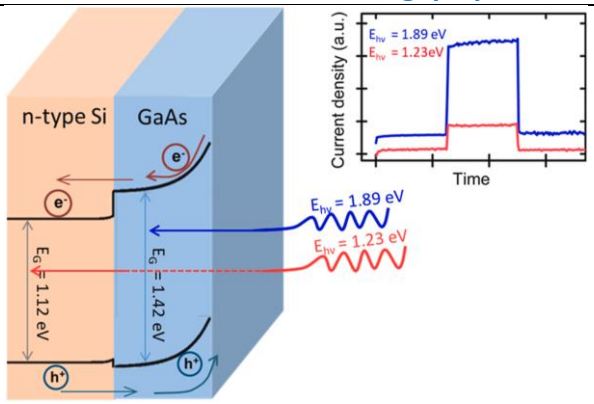
**Techniques:** *PLD, XRD, SEM-EDX*

**Materials:** $Y_1Ba_2Cu_3O_{7-\delta}$, $Mg_xZn_{1-x}O$, $Ga_2O_3$, *CuI*


**OPERA Work Group**

*WG2*

## Dual bandgap operation of a GaAs/Si photoelectrode





### Abstract

*The development of high-efficiency photoelectrodes at low manufacturing cost is of great interest for the production of renewable and green hydrogen through solar-driven water splitting. In this work, we use structural, optical, and photoelectrochemical characterizations to study the performance of unprotected epitaxial GaAs/Si photoelectrodes during photocorrosion. More specifically, we demonstrate that photoanodes including 1-µm thick GaAs epitaxially grown thin film on a low-cost Si substrate can produce a higher photocurrent than those measured for expensive commercial GaAs wafers. Based on photoelectrochemical experiments under monochromatic excitation, we show that the improved photocurrent has to be related to the dual-bandgap operation of the GaAs/Si photoelectrode, benefiting from both GaAs and Si photo-generated carriers. This result opens new possibilities to further design efficient and low-cost dual-bandgap photoelectrodes.*



*Reference:* *Solar Energy Materials and Solar Cells 251, 112138 (2023)* https://doi.org/10.1016/j.solmat.2022.112138



*Authors:* *M. Piriyev, G. Loget, Y. Léger, L. Chen, A. Létoublon, T. Rohel, C. Levallois, J. Le Pouliquen, B. Fabre, N. Bertru, C. Cornet.*

*Laboratories:* *Institut FOTON (fr), ISCR (fr).*

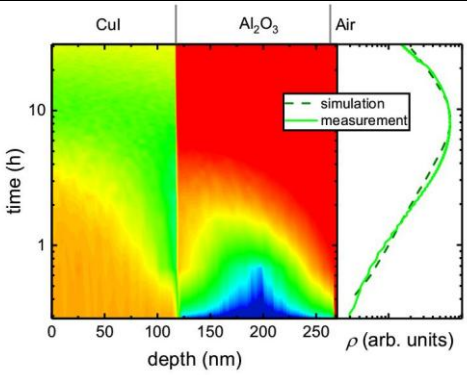

*Techniques:* *MBE, J-V PEC photoelectrochemistry.*

*Materials:* *GaAs/Si in alkaline solution.*

### OPERA Work Group

*WG2*

## Diffused Oxygen as Dominating Shallow Acceptor in p-Type Copper Iodide Thin Films





### Abstract

*The long-term stability of the optically transparent p-type semiconductor copper iodide is a current challenge. The electrical conductivity of CuI thin films depends critically on the environmental impact. $Al_2O_3$ cappings enhance the stability considerably. Systematic studies on $Al_2O_3$ / CuI heterostructures in dependence of the $N_2/O_2$ growth pressure show the electrical conductivity of the CuI films being determined by the oxygen diffusion through $Al_2O_3$ und CuI. Oxygen seems to be a dominating acceptor in CuI. We traced the diffusion of atmospheric oxygen into CuI with $^{18}O$ isotopes.*

*The Figure shows the time- and depth-resolved simulation of the diffusion of oxygen into a c-sapphire / CuI + 1at% CuO /$Al_2O_3$ hetero structure, grown in nitrogen background gas. Blue color stands for low, and red for high oxygen concentration. Right is shown the experimental and simulated electrical resistivity ρ.*



*Reference:* *Chem. Ing. Tech. 95, No. 11, 1786 ‑1793 (2023); DOI: 10.1002/cite.202300007*



*Authors:* *M. Lorenz, P. Storm, S. Gierth, S. Selle, H. von Wenckstern, M. Grundmann*

*Laboratories:* *Universität Leipzig (De), Fraunhofer Institute for Microstructure of Materials and Systems Halle (De)*

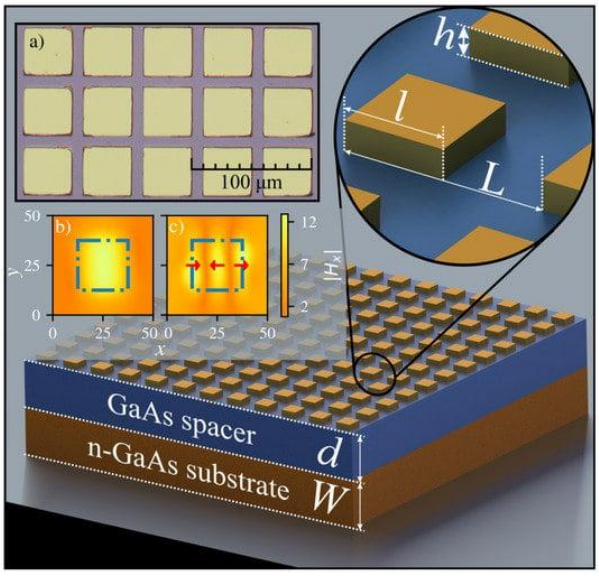

*Techniques:* *PLD, XRD, Hall effect, TOF-SIMS*

*Materials:* *CuI*

### OPERA Work Group

*WG2*

## Narrowband Thermal Terahertz Emission from Homoepitaxial GaAs Structures Coupled with Ti/Au Metasurface




*Reference:* *Sensors, Volume 23, Issue 10, 4600 (2023); https://doi.org/10.3390/s23104600*

*Authors:* *I. Grigelionis, V. Čižas, M. Karaliūnas, V. Jakštas, K. Ikamas, A. Urbanowicz, M. Treideris, A. Bičiūnas, D. Jokubauskis, R. Butkutė, L. Minkevičius*

*Laboratories:* *Optoelectronics Dept. FTMC (LT), TETI Vilnius Univ. (LT)*

*Techniques:* *MBE, thermal emission, magnetic polaritons*

*Materials:* *GaAs semiconductors, Ti/Au, metasurface*

*Abstract*

*We report on the experimental evidence of thermal terahertz (THz) emission tailored by magnetic polariton (MP) excitations in entirely GaAs-based structures equipped with metasurfaces. The* n*-GaAs/GaAs/TiAu structure was optimized using finite-difference time-domain (FDTD) simulations for the resonant MP excitations in the frequency range below 2 THz. Molecular beam epitaxy was used to grow the GaAs layer on the* n*-GaAs substrate, and a metasurface, comprising periodic TiAu squares, was formed on the top surface using UV laser lithography. The structures exhibited resonant reflectivity dips at room temperature and emissivity peaks at $T$=390 °C in the range from 0.7 THz to 1.3 THz, depending on the size of the square metacells. In addition, the excitations of the third harmonic were observed. The bandwidth was measured as narrow as 0.19 THz of the resonant emission line at 0.71 THz for a 42 μm metacell side length. An equivalent $LC$ circuit model was used to describe the spectral positions of MP resonances analytically. Good agreement was achieved among the results of simulations, room temperature reflection measurements, thermal emission experiments, and equivalent $LC$ circuit model calculations. Thermal emitters are mostly produced using a metal-insulator-metal (MIM) stack, whereas our proposed employment of* n*-GaAs substrate instead of metal film allows us to integrate the emitter with other GaAs optoelectronic devices. The MP resonance quality factors obtained at elevated temperatures ($Q$≈3.3 to 5.2) are very similar to those of MIM structures as well as to 2D plasmon resonance quality at cryogenic temperatures.*

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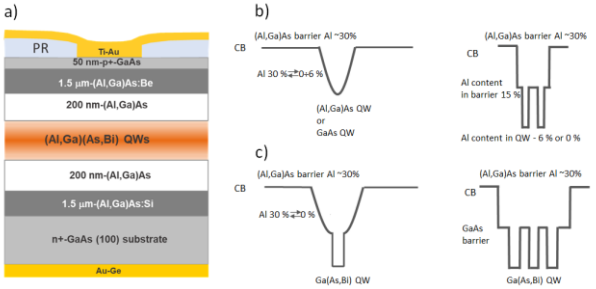
## Low-Frequency Noise Characteristics of (Al, Ga)As and Ga(As, Bi) Quantum Well Structures for NIR Laser Diodes




*Reference:* *Sensors 23, 2282 (2023) ; https://doi.org/10.3390/s23042282*

*Authors:* *S. Armalytė, J. Glemža, V. Jonkus, S. Pralgauskaitė, J. Matukas, S. Pūkienė, A. Zelioli, E. Dudutienė, A. Naujokaitis, A. Bičiūnas; B. Čechavičius, R. Butkutė*

*Laboratories:* *Optoelectronics Dept. FTMC (LT), TETI Vilnius Univ. (LT)*

*Techniques:* *MBE, MQW, PL, SEM, Noise measurement*

*Materials:* *AlGaAs, GaAsBi semiconductors*

*Abstract*

*Fabry–Perot laser diodes based on (Al, Ga)As and Ga(As, Bi) with single or multiple parabolic or rectangular-shaped quantum wells (QWs) emitting at the 780–1100 nm spectral range were fabricated and investigated for optimization of the laser QW design and composition of QWs. The laser structures were grown using the molecular beam epitaxy (MBE) technique on the* n*-type GaAs(100) substrate. The photolithography process was performed to fabricate edge-emitting laser bars of 5 μm by 500 μm in size. The temperature-dependent power-current measurements showed that the characteristic threshold current of the fabricated LDs was in the 60–120 mA range. Light and current characteristics were almost linear up to (1.2–2.0) $I_{th}$. Low-frequency 10 Hz–20 kHz electrical and optical noise characteristics were measured in the temperature range from 70 K to 290 K and showed that the low-frequency optical and electrical noise spectra are comprised of 1/f and Lorentzian-type components. The positive cross-correlation between optical and electrical fluctuations was observed.*

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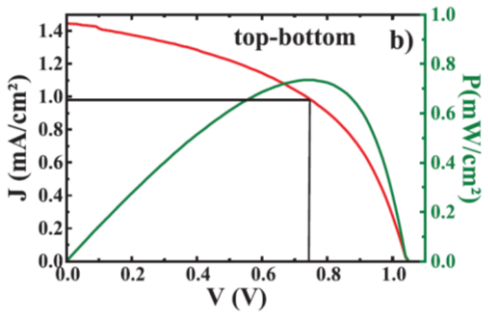
## Investigation of III-V GaP solar cell on silicon substrate




*Reference:* EPJ Photovoltaics 14, 31 (2023); DOI: https://doi.org/10.1051/epjpv/2023020

*Authors:* S. Boyer-Richard, F. Fan, A. Beck, C. Levallois, K. Tavernier, T. Rohel, R. Bernard, A. Létoublon, C. Cornet and O. Durand.

*Laboratories:* Institut FOTON (fr).

*Techniques:* MBE, I-V, EQE

*Materials:* GaP/Si

### Abstract

*The best solar conversion efficiencies have been reached thanks to multijunction solar based on III-V semiconductors on GaAs or Ge substrates. While displaying high conversion efficiencies, these solar cells suffer from the high cost of such substrates. To benefit from both the low cost and technological maturity of silicon cells, III-V tandem cells on silicon seem a good compromise to overpass the theoretical efficiency limit of the Si single cells. To study the GaP/Si interface effect on the solar cell characteristic, a GaP n-i-p solar cell has been grown on silicon substrate. Two types of electrical contacts configurations have been processed: a top-top configuration in which the current does not see the GaP/Si interface and the top-bottom configuration where the electric current crosses the interface. A comparison of dark I-V, I-V under solar illumination, and EQE measurements on both configurations is performed. The top-bottom contacts configuration shows an EQE a little bit lower than the top-top contact one, likely due to lower carrier diffusion length or recombination at the lower interface. However, the result on the EQE of the top-bottom configuration is encouraging for the future development of the GaP-based/Si tandem solar cells, and any other tandem cell on silicon using GaP as an intermediate selective contact.*

*OPERA Work Group*

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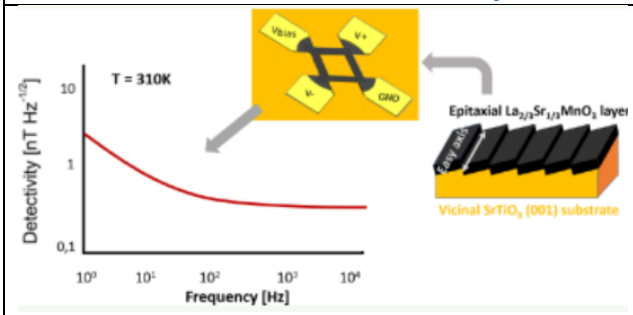
## Key Parameters for Detectivity Improvement of Low Noise Anisotropic Magnetoresistive Sensors Made of La2/3Sr1/3MnO3 Single Layers on Vicinal Substrates




*Reference:* ACS Applied Electronic Materials 2023 5 (2), 729-739 - DOI: 10.1021/acsaelm.2c01096

*Authors:* L.G. Enger, S. Flament, I.N. Bhatti, O. Rousseau, B. Guillet, M. Lam Chok Sing, V. Pierron, S. Lebargy, S. K. Chaluvadi, B. Domengés, A. Vera*, J. M. Díez, I. Martínez, R. Guerrero, L. Pérez, M.T. Gonzalez, R. Miranda, J. Camarero, P. Perna, and L. Méchin*

*Laboratories:* GREYC(Fr), IMDEA Nanociencia (ES)

*Techniques:* PLD

*Materials:* $La_{2/3}Sr_{1/3}MnO_3$

### Abstract

*The current trend in magnetoresistive sensors development is to increase the sensitivity of single sensing elements by using multilayer structures and to design them into arrays. Such arrays are designed to compensate the excess low frequency noise of individual elements, which limits their magnetic resolution. Here, we report the modeling, design, and fabrication of single layer anisotropic magnetoresistive (AMR) sensors using low noise epitaxial $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) oxide thin films deposited on vicinal $SrTiO_3$ substrates. The fabrication process is simple, and the operation of the sensor is based on a step-induced uniaxial magnetic anisotropy, described using the Stoner–Wohlfarth model. A coherent magnetization reversal process is observed by magneto-optical Kerr effect imaging. A good agreement between experimental data and the expected sensor response confirms the correct operation of the device. Three main fabrication parameters, namely the vicinal angle of the substrate, the deposition temperature, the thin film thickness, and their effects on film anisotropy field and device detectivity have been studied. Detectivity levels as low as 1.4 nT $Hz^{-1/2}$ at 1 Hz and 240 pT $Hz^{-1/2}$ in the white noise region are achieved with a single Wheatstone bridge element operating at 310 K. Compared to GMR and AMR sensors, these results are promising for further development and for their use as single layer LSMO low field AMR sensors, including applications as implantable biomedical devices.*

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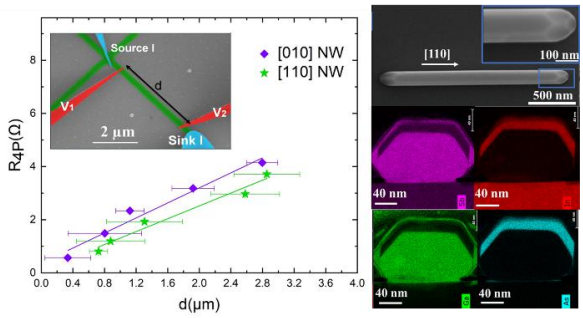
## Improving the intrinsic conductance of selective area grown in-plane InAs nanowires with a GaSb shell




*Reference:* *Nanotechnology 34 (26), 265704 (2023); doi: 10.1088/1361-6528/acc810*

*Authors:* *W Khelifi, C Coinon, M Berthe, D Troadec, G Patriarche, X Wallart, B Grandidier and L Desplanque*

*Laboratories:* *IEMN (Fr), C2N (Fr)*

*Techniques:* *MBE SAG, 4P-STM*

*Materials:* *InAs, GaSb, InP*


### Abstract

*The nanoscale intrinsic electrical properties of in-plane InAs nanowires grown by selective area epitaxy are investigated using a process-free method involving a multi-probe scanning tunneling microscope. The resistance of oxide-free InAs nanowires grown on an InP(111)B substrate and the resistance of InAs/GaSb core-shell nanowires grown on an InP(001) substrate are measured using a collinear four-point probe arrangement in ultrahigh vacuum. They are compared with the resistance of two-dimensional electron gas reference samples measured using the same method and with the Van der Pauw geometry for validation. A significant improvement of the conductance is achieved when the InAs nanowires are fully embedded in GaSb, exhibiting an intrinsic sheet conductance close to the one of the quantum well counterpart.*


### OPERA Work Group

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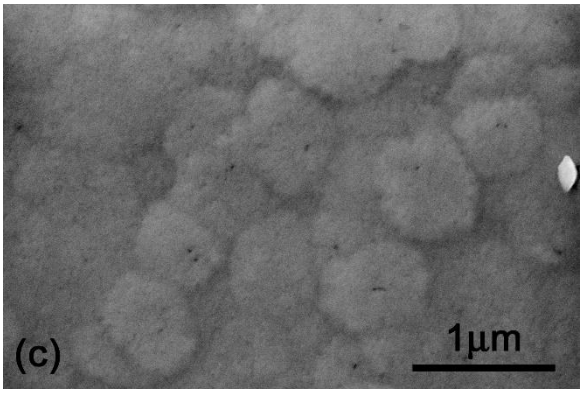
## Resistive InAlN: platform for a new type of high-speed electronics




*Reference:* *Materials, 16 (2023) 2250);* *https://www.mdpi.com/1996-1944/16/6/2250*

*Authors:* *J. Kuzmík, O. Pohorelec, S. Hasenöhrl, M. Blaho, R. Stoklas, E. Dobročka, A. Rosová, M. Kučera, F. Gucmann, D. Gregušová, M. Precner, A. Vincze.*

*Laboratories:* *Institute of Electrical Engineering (Sk), International Laser Centre, Slovak Centre of Scientific and Technical Information (Sk)*

*Techniques:* *MOCVD, AFM, SEM, TEM, XRD, Hall.*

*Materials:* *InAlN*


### Abstract

*There is a need for novel materials systems that can open a window for sub-THz-frequency electronics. Owing to its record calculated electron velocity, InN is among the hottest candidates.*

*Recent evaluation of the state-of-the art InN grown by molecular-beam-epitaxy (MBE) indicated the electron velocity of about 1 × $10^8$ $cms^{-1}$. However, experimental demonstration of InN-channel transistors is missing to date because of the large lattice misfit between InN and ordinary GaN buffers layers on which InN is normally grown. Elsewhere, it was suggested that InAlN buffer layers with a high In content could resolve this issue by providing better matching.*

*In our work, we studied Mg-doping of In-rich InAlN layers by using MOCVD with varied $CP_2Mg$ flow between 0 and 130 nmol/min. We concluded that by Mg-doping of the In-rich InAlN, mobility of free electrons is the main factor which controls the material resistivity. In future, Mg-doped InAlN material can be tested for the buffer layer in the design of novel InN/InAlN transistor structures.*


### OPERA Work Group

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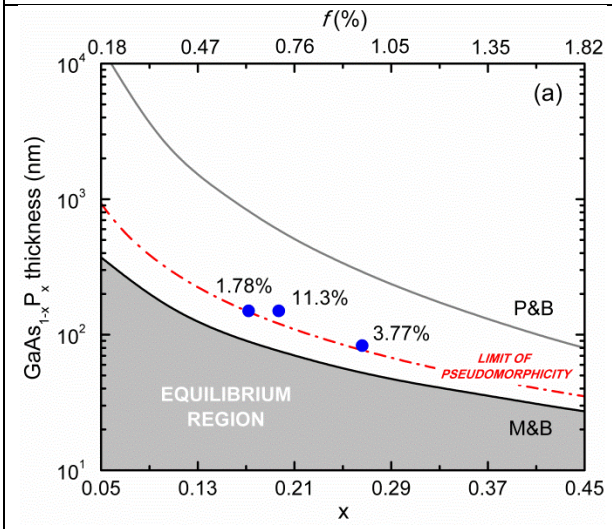
## Lattice Strain Relaxation and Compositional Control in As-Rich GaAsP/(100)GaAs Heterostructures Grown by MOVPE




*Reference:* *Materials 16 (2023) 4254. DOI : 10.3390/ma16124254*

*Authors:* *P. Prete, D. Calabriso, E. Burresi, L. Tapfer , N. Lovergine*

*Laboratories:* *IMM-CNR (It), Univ. Salento (It)*

*Techniques:* *MOCVD, XRD, FESEM.*

*Materials:* *GaAsP, GaAs*

### Abstract

*The fabrication of high-efficiency GaAsP-based solar cells on GaAs wafers requires to address structural issues arising from the materials lattice mismatch. We report on tensile strain relaxation and composition control of MOVPE-grown As-rich $GaAs_{1-x}P_x$/(100)GaAs heterostructures studied by double-crystal X-ray diffraction and field emission scanning electron microscopy. Thin (80–150 nm) $GaAs_{1-x}P_x$ epilayers appear partially relaxed (within 1–12% of the initial misfit) through a network of misfit dislocations along the sample [011] and [011] in plane directions. Values of the residual lattice strain as function of epilayer thickness were compared with predictions from the equilibrium (Matthews–Blakeslee) and energy balance models. It is shown that the epilayers relax at a slower rate than expected based on the equilibrium model, an effect ascribed to the existence of an energy barrier to the nucleation of new dislocations. The study of $GaAs_{1-x}P_x$ composition as a function of the V-group precursors ratio in the vapor allowed the determination of the As/P anion segregation coefficient. The latter agrees with values reported in the literature for P-rich alloys grown using the same precursor combination. P-incorporation into nearly pseudomorphic heterostructures turns out to be kinetically activated, with an activation energy $E_A$ = 1.41 ± 0.04 eV over the entire alloy compositional range.*

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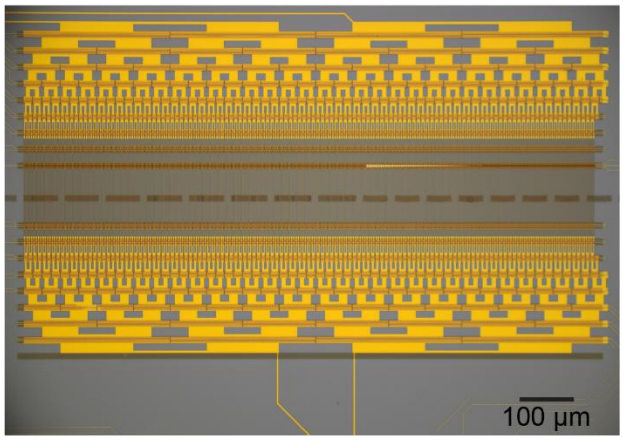
## Cryogenic Multiplexing Using Selective Area Grown Nanowires




*Reference:* *Nat. Commun. 14, 7738 (2023); doi: 10.1038/s41467-023-43551-1*

*Authors:* *D. Olšteins, G. Nagda, D. J. Carrad, D. V. Beznasyuk, C. E. N. Petersen, S. Martí-Sánchez, J. Arbiol, T. S. Jespersen*

*Laboratories:* *Center for Quantum Devices KU (dk), Department of Energy Conversion and Storage DTU (dk), ICN2 (es), ICREA (es)*

*Techniques:* *MBE, EBL, electrical measurements*

*Materials:* *InAs, GaAs semiconductors*

### Abstract

*Bottom-up grown nanomaterials play an integral role in the development of quantum technologies but are often challenging to characterise on large scales. Here, we harness selective area growth of semiconductor nanowires to demonstrate large-scale integrated circuits and characterisation of large numbers of quantum devices. The circuit consisted of 512 quantum devices embedded within multiplexer/demultiplexer pairs, incorporating thousands of interconnected selective area growth nanowires operating under deep cryogenic conditions. Multiplexers enable a range of new strategies in quantum device research and scaling by increasing the device count while limiting the number of connections between room-temperature control electronics and the cryogenic samples. As an example of this potential we perform a statistical characterization of large arrays of identical quantum dots thus establishing the feasibility of applying cross-bar gating strategies for efficient scaling of future selective area growth quantum circuits. More broadly, the ability to systematically characterise large numbers of devices provides new levels of statistical certainty to materials/device development.*

### OPERA Work Group

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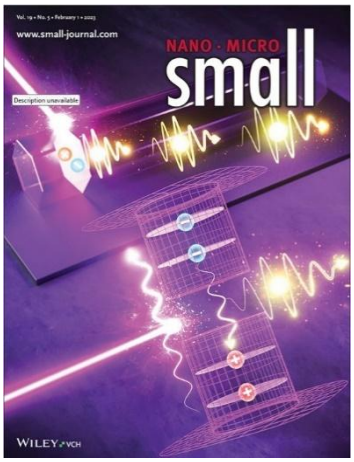
## Enhancement of Single-Photon Purity and Coherence of III-Nitride Quantum Dot with Polarization-Controlled Quasi-Resonant Excitation




*Reference:* *Small 19, 2205229 (2023); doi:10.1002/smll.202205229*

*Authors:* *S. Jun, M. Choi, B. Kim, M. Morassi, M. Tchernycheva, H. G. Song, H-S Yeo, N. Gogneau, Y-H. Cho.*

*Laboratories:* *Department of Physics and KI for the NanoCentury, KAIST (Republic of Korea), C2N/CNRS/Paris-Saclay Univ. (Fr).*

*Techniques:* *PA-MBE, quasi-resonant excitation (QRE) method.*

*Materials:* *Axial InGaN/GaN Nanowires*

### Abstract

*III-Nitride semiconductor-based quantum dots (QDs) play an essential role in solid-state quantum light sources because of their potential for room-temperature operation. However, undesired background emission from the surroundings deteriorates single-photon purity. Moreover, spectral diffusion causes inhomogeneous broadening and limits the applications of QDs in quantum photonic technologies. To overcome these obstacles, it is demon-strated that directly pumping carriers to the excited state of the QD reduces the number of carriers generated in the vicinities. The polarization-controlled quasi-resonant excitation is applied to InGaN QDs embedded in GaN nano-wire. To analyze the different excitation mechanisms, polarization-resolved absorptions are investigated under the above-barrier bandgap, below-barrier bandgap, and quasi-resonant excitation conditions. By employing polari-zation-controlled quasi-resonant excitation, the linewidth is reduced from 353 to 272 μeV, and the second-order correlation value is improved from 0.470 to 0.231. Therefore, a greater single-photon purity can be obtained at higher temperatures due to decreased linewidth and background emission.*

### OPERA Work Group

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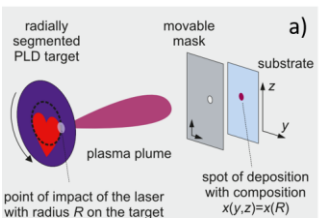
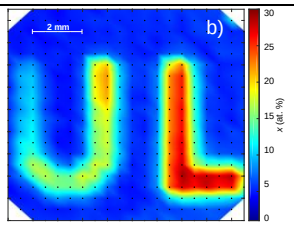
## MARS-PLD: A Novel Method for Area-Selective Deposition using Pulsed-Laser Deposition




*Reference:* *J. Vac. Sci. Technol. A 41, 020801 (2023); DOI: https://doi.org/10.1116/6.0002275*

*Authors:* *L. Thyen, D. Splith, M. Kneiß, M. Grundmann, H. von Wenckstern*

*Laboratories:* *Universität Leipzig (De)*

*Techniques:* *PLD, XRD, SEM-EDX*

*Materials:* $Mg_xZn_{1-x}O$

### Abstract

*A novel area-selective deposition approach based on Pulsed Laser Deposition allows the growth of arbitrary material patterns on a substrate and, in addition, allows for the precise control of chemical composition at the μm scale. The method, schematically illustrated in figure a), combines the ablation of radially segmented targets with an independently movable shadow mask in front of the substrate with a spatial resolution of about 10 μm. This method is denoted as mask-assisted radially-segmented target PLD (MARS-PLD). As an illustration of combining area-selective deposition with a material gradient results of an energy-dispersive X-ray spectroscopy mapping is shown in figure b) in a false color representation for a (Mg,Zn)O realized by MARS-PLD. We used a shadow mask with a 1 × 1 mm² notch to create a (Mg,Zn)O graded pattern of the letters "U" and "L" (Universität Leipzig).*

### OPERA Work Group

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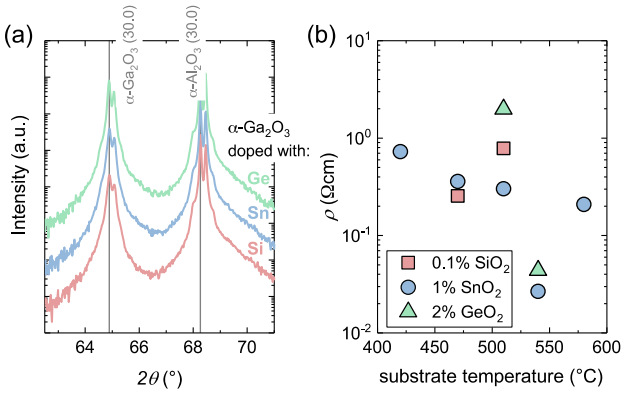
## Realization of conductive n-type doped α-$Ga_2O_3$ on m-plane sapphire grown by a two-step pulsed laser deposition process




*Reference:* *Phys. Status Solidi A, 220: 2200721 (2023);*
*DOI: https://doi.org/10.1002/pssa.202200721*

*Authors:* *S. Vogt, C. Petersen, M. Kneiß, D. Splith, T. Schultz, H. von Wenckstern, N. Koch, M. Grundmann*

*Laboratories:* *Universität Leipzig (De)*

*Techniques:* *PLD, XRD, van der Pauw*

*Materials:* *$Ga_2O_3$*

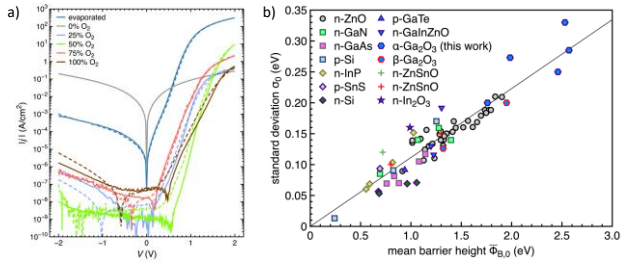
### Abstract

*$Ga_2O_3$ is highly promising for high-power transistors and solar blind photo-detectors due to its wide bandgap. It crystallizes in different polymorphs, of which the monoclinic β-polymorph is thermodynamically stable, but the rhombohedral α-phase has the highest bandgap of about 5.3eV and thus the highest expected electric breakdown field. α-$Ga_2O_3$ can be grown on isostructural α-$Al_2O_3$ substrates, however, the growth of conductive thin films remains challenging. We fabricated conductive α-Ga2O3 thin films by pulsed laser deposition on an optimized high-temperature α-$Ga_2O_3$ buffer with a thickness of 75 nm. The conductive thin films were doped with tin, silicon or germanium at different growth temperatures between 420°C and 580°C. In Figure a), X-ray diffractograms of three thin films deposited at 540°C are depicted. A (10.0) oriented α-$Ga_2O_3$ growth is verified for all three dopants. The crystal quality is very similar for all three dopants at this growth. Investigations on the electrical properties yielded that tin-doped thin films had the widest growth temperature. For germanium and silicon doping, the growth window was much narrower. Tin doping also yielded the lowest resistivity of $\rho = 2.7 \times 10^{-2}$ Ωcm as shown in Figure b). The deposition of conductive thin films discloses the possibility of using PLD for the fabrication of α-$Ga_2O_3$ demonstrator devices.*

### OPERA Work Group

*WG2*

## Properties of Schottky barrier diodes on heteroepitaxial α-$Ga_2O_3$ thin films




*Reference:* *J. Vac. Sci. Technol. A 41, 043411 (2023);*
*DOI: https://doi.org/10.1116/6.0002651*

*Authors:* *S. Köpp, C. Petersen, D. Splith, M. Grundmann, H. von Wenckstern*

*Laboratories:* *Universität Leipzig (De)*

*Techniques:* *PLD, Sputtering, Current-Voltage Measurements*

*Materials:* *$Ga_2O_3$*

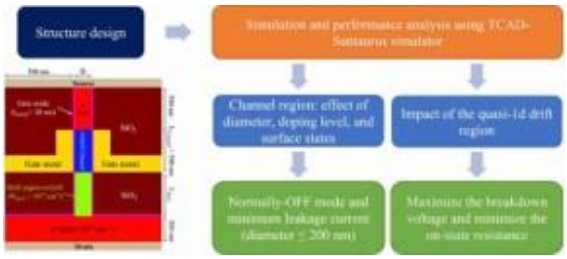
### Abstract

*$Ga_2O_3$ is emerging as a viable alternative to GaN or SiC for the fabrication of high-power electronic devices. We have compared the electrical parameters of sets of Schottky barrier diodes (SBD) fabricated by different deposition methods and using different metals on heteroepitaxial α-Ga2O3:Sn thin films. For platinum contacts, we compared the properties of non-oxidized contacts realized by thermal evaporation or inert sputtering to oxidized SBDs fabricated by reactive sputtering. For the oxidized contacts, we additionally changed the volume flow ratio of oxygen and argon $O_2$/Ar between 25%/75% and 100%/0%. Room temperature current-density-voltage (jV) characteristics of typical non-oxidized and oxidized Pt/α-Ga2O3 diodes are depicted in Figure a). The lowest reverse current densities are obtained for oxidized SBDs and sets of diodes realized with 25%/75% and 50%/50% O2/Ar volume flow ratio show on average highest current rectification. The homogeneous barrier height and its standard deviation were determined from temperature-dependent jV measurements and the results are compared to literature data in Figure b) indicating that the empirical Lajn's rule is also valid for Ga2O3 -based Schottky barrier diodes.*

### OPERA Work Group

*WG2*

## Design, Simulation and Optimization of an Enhanced Vertical GaN Nanowire Transistor on Silicon Substrate for Power Electronic Applications




*Reference:* *IEEE Access, Volume 11, 40249 (2023); doi: 10.1109/ACCESS.2023.3248630*

*Authors:* *M. Benjelloun, Z. Zaidan, A. Soltani, N. Gogneau, D. Morris, J-C Harmand, H. Maher.*

*Laboratories:* *LN2/CNRS IRI/Sherbrooke Univ. (Canada), C2N/CNRS/Paris-Saclay Univ. (Fr).*

*Techniques:* *TCAD-Santaurus tool*

*Materials:* *GaN Nanowires*

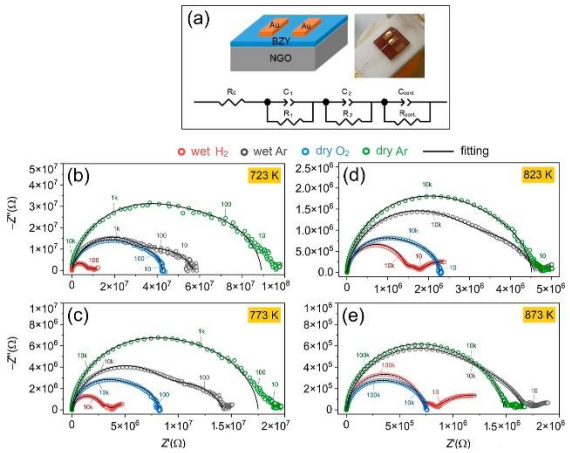
### *Abstract*

*A new vertical transistor structure based on GaN nanowire is designed and optimized using the TCAD-Santaurus tool with an electrothermal model. The studied structure with quasi-1D drift region is adapted to GaN nanowires synthesized with the bottom-up approach on a highly n-doped silicon substrate. The electrical performance is studied as a function of various epi-structure parameters, including region lengths and doping levels, nanowire diameter, and the impact of the surface states. The results reveal that the optimized structure has a Normally-OFF mode with a threshold voltage higher than 0.8 V and exhibits minimized leakage current, low on-state resistance, and maximized breakdown voltage. To the best of our knowledge, this is the first exhaustive study of GaN-based nanowire transistors, providing valuable insights for the scientific community and contributing to a deeper understanding of the impact of GaN nanowire parameters on device performance.*

### *OPERA Work Group*

*WG2*

## The Role of Strain in Proton Conduction in Multi-Oriented $BaZr_{0.9}Y_{0.1}O_{3-\delta}$ Thin Film




*Reference:* *ACS Appl. Mater. Interfaces 2022, 14, 50, 55915–55924* *https://doi.org/10.1021/acsami.2c12657*

*Authors:* *M. Shahrukh Saleem, Q. Chen, N. A. Shepelin, S. Dolabella, M. D. Rossell, X. Zhang, C. X. Kronawitter, F. La Mattina, and A. Braun*

*Laboratories:* *Empa (CH), UMich Joint Institute Shanghai Jiao Tong University (PRC), PSI (CH), Southeast University (PRC), UC Davis (USA)*

*Techniques:* *PLD, XRD, TEM, Impedance spectroscopy*

*Materials:* *BZY, (110) NdGaO3*

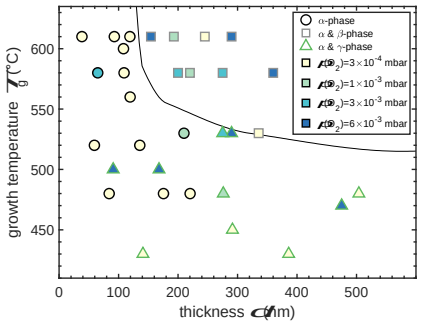
### *Abstract*

*Within the emerging field of proton-conducting fuel cells, yttrium substituted barium zirconate (BZY10) is an attractive material due to its high conductivity and stability. The fundamentals of conduction in sintered pellets and thin films heterostructures have been explored; but the role of crystallographic orientation, grains, and grain boundaries is poorly understood for proton conduction. This article reports proton conduction in multioriented BZY10 thin film grown on top of a (110) NdGaO3 substrate. The multiple orientations are composed of different lattices, which provide a platform to study the lattice-dependent conductivity through different orientations in the vicinity of grain boundary between them and the substrate. The crystalline stacking of each orientation is confirmed by X-ray diffraction analysis and scanning transmission electron microscopy. The transport measurements are carried out under different atmospheres. The highest conductivity is found under a wet H2 environment together with an increased lattice parameter of 4.208 A, while under O2 and Ar environment, the film shows lower conductivity and smaller lattice parameter. Our findings demonstrate the role of crystal lattice for conduction properties and illustrate the importance of self-assembled strategies to achieve high proton conduction in BZY10 thin films.*

### *OPERA Work Group*

*WG2*

## PLD of α-$Ga_2O_3$ on m-plane $Al_2O_3$: Growth regime, growth process, and structural properties




*Reference:* *APL Mater. 11, 061122 (2023);*
*DOI: https://doi.org/10.1063/5.0149797*

*Authors:* *C. Petersen, S. Vogt, M. Kneiß, H. von Wenckstern, M. Grundmann*

*Laboratories:* *Universität Leipzig (De)*

*Techniques:* *PLD, XRD, AFM*

*Materials:* *$Ga_2O_3$*

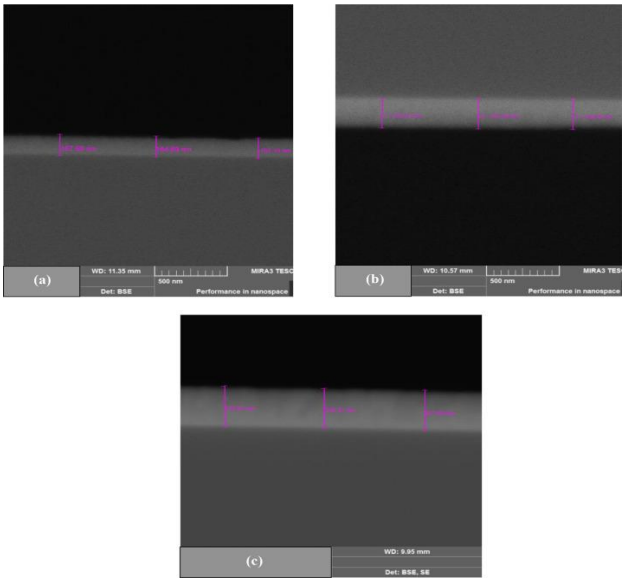
### Abstract

*The growth of $Ga_2O_3$ on m-plane sapphire was comprehensively studied using pulsed laser deposition. A distinct growth regime for the α-$Ga_2O_3$ phase was identified, and optimal growth conditions for phase-pure α-$Ga_2O_3$ with superior crystal quality and low surface roughness were determined. By varying the oxygen partial pressure and the layer thickness at different fixed substrate temperatures, we were able to construct a complex phase diagram (shown in the figure) with a distinct growth regime in favor of α-$Ga_2O_3$. Low oxygen pressure and growth temperatures above 450°C result in phase-pure (10.0)-oriented α-$Ga_2O_3$ layers without rotational domains. Samples with the highest crystallinity have the lowest so far reported full-width at half maximum of the (30.0)-peak in rocking curves of 960" together with an exceptionally low surface roughness of 0.7 nm (RMS). The knowledge on the growth of α-$Ga_2O_3$ on $Al_2O_3$ substrates gained in this study is essential to fabricating cost-effective high-performance demonstrator power devices.*

### OPERA Work Group

*WG2*

## Comprehensive growth and characterization study of GeOx/Si




*Reference:* *Journal of Molecular Structure, 1274, 134398 (2023); doi; 10.1016/j.molstruc.2022.134398*

*Authors:* *Baghdedi D, Hopoğlu H, Sarıtaş S, Demir İ, Altuntaş İ, Abdelmoula N, Gür E, Tüzemen EŞ.*

*Laboratories:* *The Nanophotonics Research and Application Center at Sivas Cumhuriyet University (CUNAM) (Tr), Sivas Cumhuriyet University R&D Center (CUTAM) (Tr), and Laboratory of Multifunctional Materials and Applications (LaMMA), at University of Sfax (Tn)*

*Techniques:* *Radio frequency (RF) magnetron sputtering, XRD, SEM, UV- VIS-NIR Spectrophotometer, and Spectroscopic Ellipsometry*

*Materials:* *$GeO_2$*

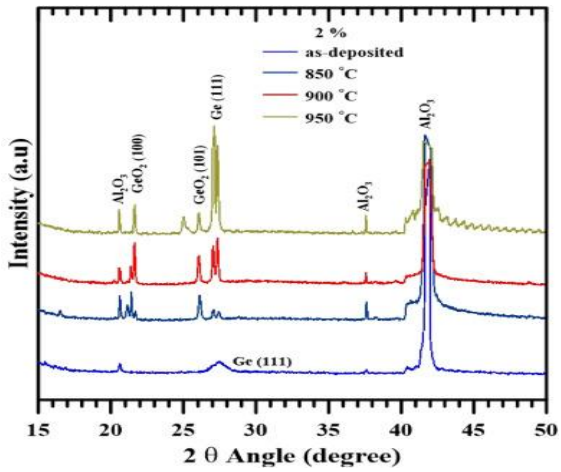
### Abstract

*In this study, the reactive radio frequency magnetron sputtering (RFMS) method under varying thickness was used to deposit GeOx on Si substrate at room temperature. The effect of thickness on the structural and optical properties of high-quality germanium dioxide ($GeO_2$) thin films have been investigated by experimental. Structural properties were investigated using X-ray diffraction. It has been observed that the peak intensity of (113) reflection is the highest in the spectrum of 240.22 nm thickness and using scanning electron microscope (SEM) to calculate thickness of different samples. Reflection measurement, which is one of its optical properties, was measured with an optical spectrophotometer. It has been observed that as the thickness increases, the total reflectance changes. The absorption coefficient was calculated using the diffuse reflection curve. From this point of view, the energy band gap was calculated, and it was seen that it varies between 4.1 eV and 4.4 eV. As a result, it was observed that the energy band gap increased as the thickness increased. And using spectroscopic ellipsometry to calculate the thickness of different, refractive index, extinction coefficient, and oscillator parameters. The oscillator energy decrease as the thickness of films increases and the dispersion energy increase with the increase of thickness. It has been observed that the thickness varies between 174.29 nm and 332.16 nm. The refractive index increases as the thickness increases.*

### OPERA Work Group

*WG2*

## Experimental and theoretical insights on the structural and optical properties of GeOx thin films deposited via RF magnetron sputtering under varying oxygen percentage




*Reference:* *Physica B: Condensed Matter, 650, 414494 (2023); doi; 10.1016/j.physb.2022.414494*

*Authors:* *Tüzemen EŞ, Hopoğlu H, Sarıtaş S, Aydınoğlu HS, Ertuğrul M, Maslov MM, Kaya S, Ungan F, and Gür E*

*Laboratories:* *The Nanophotonics Research and Application Center at Sivas Cumhuriyet University (CUNAM) (Tr), and Sivas Cumhuriyet University R&D Center (CUTAM) (Tr)*

*Techniques:* *RFMS, XRD, UV-VIS-NIR Spectro-photometer, and FTIR*

*Materials:* *$GeO_2$*

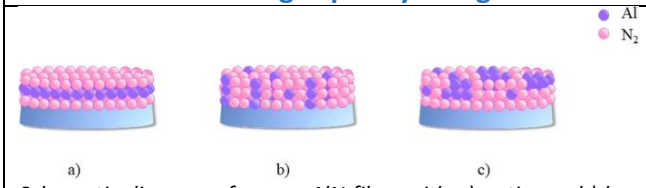
### Abstract

*In this study, GeOx films were produced by radio frequency magnetron sputtering (RFMS) under varying oxygen percentages. The structural and optical properties of films grown have been studied experimentally and theoretical calculations have been presented using density functional theory (DFT). Considering the x-ray diffraction (XRD) analysis, Ge (111) peak was observed in the as-deposited film produced only at 2% oxygen percentage. In order to emerge crystal phases, all the amorphous films were annealed at 900 °C under atmospheric conditions. It was found that the intensity of the (101) peak increased as the oxygen percentage increased. At the same time, film grown at 2% oxygen percentage was annealed at different annealing temperatures sequentially at 850, 900, and 950 °C. As a result, the polycrystalline properties changed as the annealing temperature increased. It was found that the optical properties of the films grown are strongly dependent on the oxygen percentage. As the oxygen percentage has changed, the energy band gap has increased to the values 2.30, 2.31, 2.58, and 6.28 eV. There are Ge-O-Ge antisymmetric stretching peaks appeared at 861.51 cm−1, 949.94 cm−1 and symmetric stretching of hexagonal peaks at 516.34 cm−1, 546.29 cm−1, 581.95 cm−1. The energy band gap results of the density functional theory (DFT) calculations are in good agreement with the experimental observations.*

*OPERA Work Group*

*WG2*

## High-quality AlN growth: a detailed study on ammonia flow




*Schematic diagram of grown AlN films with a) optimum b) low and c) high NH3 flow rate*

*Reference:* *Journal of Materials Science: Materials in Electronics, 34(4), 250 (2023); doi; 10.1007/s10854-022-09556-0*

*Authors:* *Yolcu, G., Koçak, M. N., Ünal, D. H., Altuntas, I., Horoz, S., and Demir, I.*

*Laboratories:* *The Nanophotonics Research and Application Center at Sivas Cumhuriyet University (CUNAM) (Tr),*

*Techniques:* *MOVPE, AFM, HRXRD, UV- VIS-NIR Spectrophotometer, and Raman*

*Materials:* *AlN/Sapphire*

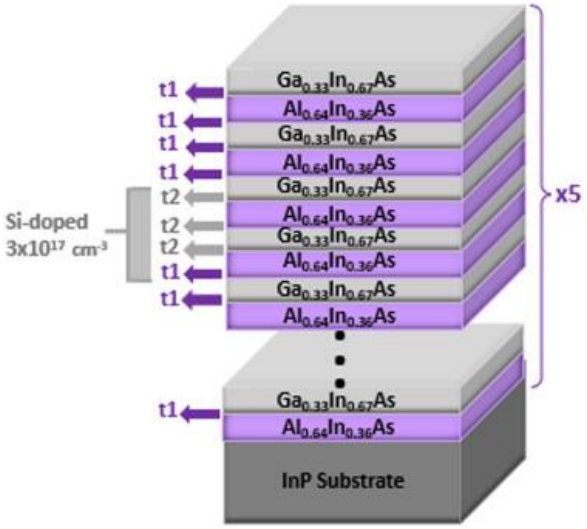
### Abstract

*High crystalline and optical quality aluminum nitride (AlN) films with thin thickness have been grown on Al2O3 by MOVPE (metal-organic vapor phase epitaxy) and the NH3 flow rate has been changed to improve the morphology and quality of the films. Some characterization types of equipment such as atomic force microscopy (AFM), high-resolution X-ray diffraction (HRXRD), and Raman spectroscopy have been carried out to investigate the effect of different NH3 flow rates on surface morphology, roughness, and crystal quality of AlN, respectively. Unlike in the literature, in situ optical reflectance measurements have been given depending on NH3 flow rate and optical characterization has been performed by UV–VIS–NIR spectrophotometry. The well-defined interference patterns in the optical transmittance graph report a sharp interface between AlN and Al2O3. Also, all obtained samples have a sharp absorption edge that shows the quality of the films, but Sample B with 900 sccm NH3 flow has the sharpest absorption edge because it has high optical quality and low defect. The RMS (root mean square), $D_S$ (screw-type dislocation density), and $D_E$ (edge-type dislocation density) values of AlN with 900 sccm NH3 flow are 0.22 nm, 7.86 x 107, and 1.68 x 1010 cm−2, respectively. The results obtained are comparable to the literature.*

*OPERA Work Group*

*WG2*

## Effect of Si-doped and undoped inter-layer transition time on the strain-compensated InGaAs/InAlAs QCL active region grown with MOVPE




*Reference:* *Journal of Molecular Structure, 1272, 134203 (2023); doi; 10.1016/j.molstruc.2022.134203*

*Authors:* *Perkitel, I., and Demir, I.*

*Laboratories:* *The Nanophotonics Research and Application Center at Sivas Cumhuriyet University (CUNAM) (Tr)*

*Techniques:* *MOVPE, and HRXRD*

*Materials:* *InGaAs/InAlAs*


### Abstract

*In this study, we report the effect of the combination of Si-doped and undoped inter-layer transition time in the strain compensated In0.67Ga0.33As/In0.36Al0.64As quantum cascade laser (QCL) structure grown on InP substrate by Metal Organic Vapor Phase Epitaxy (MOVPE). In situ reflectance spectroscopy and high-resolution X-ray diffraction (HRXRD) technique have been used for the analysis of growth steps and crystalline quality of QCL structures, respectively. In addition, since thickness accuracy is very important for QCLs, two different thickness calculation methods have been used in the Global Fit simulation program for detailed thickness accuracy of structures. As a result, optimum values for thickness accuracy have been obtained as 5 and 10 s between undoped and Si-doped layers, respectively, as verified by the two methods.*


*OPERA Work Group*

*WG2*

## InGaAs-Based MSM Photodetector: Researching Absorption Layer, Barrier Layer, and Digital Graded Superlattice Layer with 3D Simulation

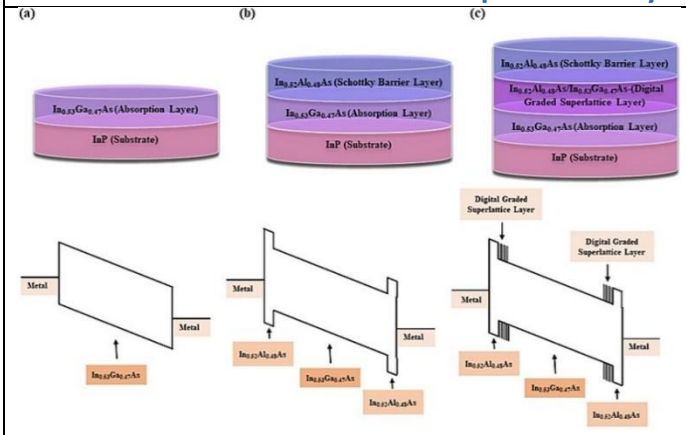



*Fig. 1. (a) Study A structure and bandgap under reverse voltage; (b) Study B structure and bandgap under reverse voltage; (c) Study C structure and bandgap under reverse voltage*

*Reference:* *Results in Optics, 100581 (2023); doi; 10.1016/j.rio.2023.100581*

*Authors:* *Unal DH, Demir I.*

*Laboratories:* *The Nanophotonics Research and Application Center at Sivas Cumhuriyet University (CUNAM) (Tr)*

*Techniques:* *Silvaco TCAD software*

*Materials:* *InGaAs, InAlAs, InP*

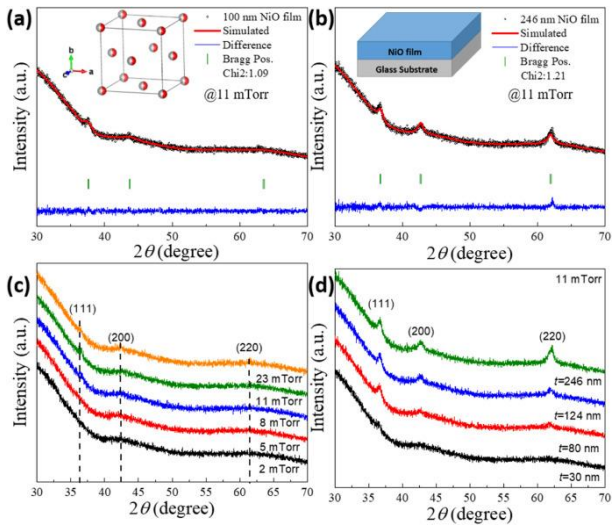

### Abstract

*The effects of absorption, barrier, and digital graded layer thickness on dark current and photocurrent in Metal Semiconductor Metal (MSM) photodetectors by using 3D Silvaco TCAD are reported. The photo-dark current ratio ($I_{photo}/I_{dark}$) is calculated using the photocurrent and dark current values obtained by simulation. In study A (absorption layer thickness variation) the photocurrent, dark current and photo-dark current ratio are increased with increased absorption layer thickness, and the dark current is 1.138x10$^{-7}$ A levels. In Study B (barrier layer thickness variation), when the barrier layer is added to the absorption layer, the dark current is decreased to 1.56x10$^{-11}$ A levels. It is reported that the photo-dark current ratio with increasing barrier layer thickness increases. In study C (digital graded superlattice layer thickness variation), the dark current increases, and photocurrent decreases with the increase of the digital graded superlattice layer thickness. However, the photo-dark current ratio with increasing digital graded superlattice layer thickness decreases. Furthermore, a similar trend of development is observed on photo-dark current with adding of the barrier layer and digital graded superlattice layer on the absorption layer. These findings demonstrate the importance of optimizing layer thickness in MSM photodetectors for improved device performance.*


*OPERA Work Group*

*WG2*

## Investigating the optical, electronic, magnetic properties and DFT of NiO films prepared using RF sputtering with various argon pressures




*Reference:* *Physica B: Condensed Matter 661: 414937 (2023); doi; 10.1016/j.physb.2023.414937*

*Authors:* *Hopoğlu, H., Kaya, D., Maslov, M. M., Kaya, S., Demir, İ., Altuntaş, İ., Ungan, F., Akyol, M., Ekicibil, A., and Tüzemen, E. Ş.*

*Laboratories:* *The Nanophotonics Research and Application Center at Sivas Cumhuriyet University (CUNAM) (Tr), and Sivas Cumhuriyet University R&D Center (CUTAM) (Tr)*

*Techniques:* *RF magnetron sputtering (MS), XRD, Hall, AFM, SEM, and UV- VIS-NIR Spectrophotometer*

*Materials:* *$NiO/SiO_2$*

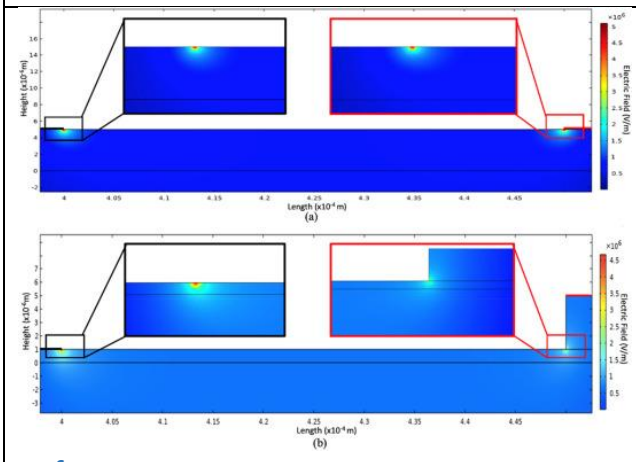

### Abstract

*In this study, we investigated the structural, optical, magnetic, and conductive properties of nickel oxide (NiO) films on glass substrates deposited using Radio Frequency (RF) magnetron sputtering with varying Ar gas pressure and thickness. X-ray diffraction and Rietveld refinement analysis confirmed a cubic crystal structure and showed that the lattice parameters and the d (111)-space increased from 4.0559 Å to 4.2712 Å and from 2.3208 Å to 2.4582 Å, respectively, due to increased Ar pressure during deposition. Scanning electron microscopy and atomic force microscopy were used to determine the cross-sectional and surface topology of the NiO films, which exhibited uniform and homogeneous growth with an average spherical size of 54.28 ± 0.33 nm. The optical bandgap values of the films were calculated to be between 3.26 and 3.65 eV, increasing with pressure. Hall measurements confirmed the p-type semiconductor nature of the films with an average sheet carrier density of 1010 cm−2. The films exhibited soft magnetic properties, with a maximum Hc and Ms of 178.5 Oe and 5.82 emu/cm3 for 246 nm NiO film, respectively. Density functional theory (DFT) calculations confirmed the experimental results for both single to five layers NiO films and bulk NiO formations. The refined energy gap value was found to be 3.2 eV by the DFT calculation. The films produced at room temperature were found to be stable and reproducible, making them suitable as p-type materials for device construction.*


### OPERA Work Group

*WG2*

## InGaAs-based Gunn light emitting diode




*Reference:* *Materials Science in Semiconductor Processing, 159, 107389 (2023); doi; 10.1016/j.mssp.2023.107389*

*Authors:* *Kalyon, G., Mutlu, S., Kuruoglu, F., Pertikel, I., Demir, I., and Erol, A*

*Laboratories:* *The Nanophotonics Research and Application Center at Sivas Cumhuriyet University (CUNAM) (Tr)*

*Techniques:* *MOVPE, XRD, Hall, Photolithography, Electroluminescence (EL), PL, and High voltage pulse generator*

*Materials:* *InGaAs/InP*

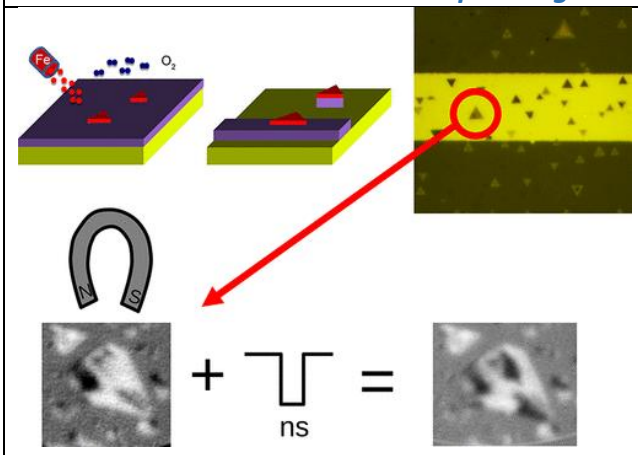

### Abstract

*We report an n-type In0.53Ga0.47As based Gunn light emitting diode operated at around 1.6 μm. The device structure comprises of an n-type In0.53Ga0.47As epilayer with a thickness of 5 μm grown by Metal Organic Vapour Phase Epitaxy (MOVPE) on a semi-insulating InP substrate and fabricated in a planar architecture with a stepped structure at anode side to suppress the destructive effect of high built-in electric field in propagating Gunn domain. Gunn diode is operated under pulsed voltage with a pulse width of 60 ns and pulse duration of 4.5 ns to keep the duty cycle as low as 0.0013%. The Gunn oscillations with an 1 ns period are observed at around 4.1 kV/cm, which corresponds to the electric field threshold of Negative Differential Resistance (NDR). The light emission at around 1.6 μm also starts at the threshold electric field of the NDR region (E = 4.2 kV/cm) of the current-voltage curve, and the emission intensity increases drastically with increasing applied electric field. The observed light emission at NDR threshold electric field where Gunn oscillations appear on the voltage pulse is attributed to the impact ionisation process occurring in the current domains along the sample, which generates excess carriers to initiate the band-to-band recombination in In0.53Ga0.47As.*


### OPERA Work Group

*WG2&3*

## *A Platform for Addressing Individual Magnetite Islands Grown Epitaxially on Ru(0001) and Manipulating Their Magnetic Domains*




*Reference:* *Cryst. Growth Des. 23, 5785 (2023), doi: 10.1021/acs.cgd.3c00388*

*Authors:* *S. Ruiz-Gómez, E.M. Trapero, C. Fernández-González, A. del Campo, C. Granados-Miralles, J.E. Prieto, Muhammad Waqas Khaliq, M.A. Niño, M. Foerster, L. Aballe, and J. de la Figuera*

*Laboratories:* *Instituto de Química Física Blas Cabrera (ES), Alba Synchrotron Light Facility (ES), Instituto de Cerámica y Vidrio (ES), Universidad Complutense de Madrid (ES)*

*Techniques:* *Magnetron sputtering, MBE*

*Materials:* *Oxides*

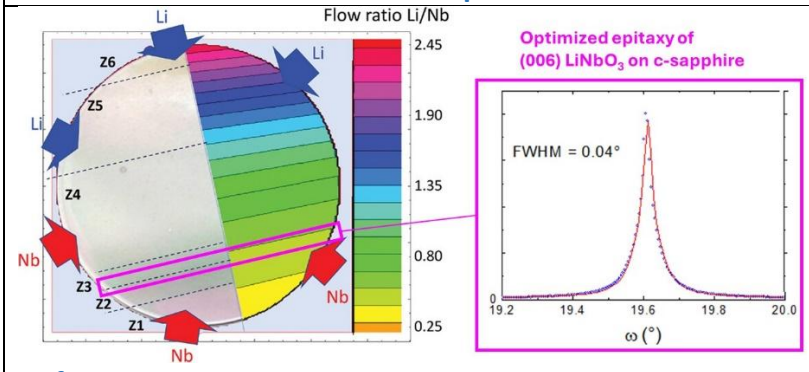

### *Abstract*

*In this work, we have grown high-quality magnetite micrometric islands on ruthenium stripes on sapphire through a combination of magnetron sputtering (Ru film), high-temperature molecular beam epitaxy (oxide islands), and optical lithography. The samples have been characterized by atomic force microscopy, Raman spectroscopy, X-ray absorption and magnetic circular dichroism in a photoemission microscope. The magnetic domains on the magnetite islands can be modified by the application of current pulses through the Ru stripes in combination with magnetic fields. The modification of the magnetic domains is explained by the Oersted field generated by the electrical current flowing through the stripes underneath the magnetite nanostructures. The fabrication method is applicable to a wide variety of rock salt and spinel oxides.*


*OPERA Work Group*

*WG2*

## Title: Efficient Optimization of High-Quality Epitaxial Lithium Niobate Thin Films by Chemical Beam Vapor Deposition: Impact of Cationic Stoichiometry




*Reference:* *Adv. Mater. Interfaces 2023, 2300535. DOI: 10.1002/admi.202300535*

*Authors:*. *A.L. Pellegrino, E. Wagner, F. Lo Presti, W. Maudez, S. Kolb, R. Rani, A. Bernard, S. Guy, A. Gassenq, M. Raevskaia, C. Grillet, R. Moalla, C. Botella, R. Bachelet, B. Masenelli, J.-M. Bluet, S. Cueff, P. Chapon, G. Benvenuti, G. Malandrino*

*Laboratories:* *3D-Oxides (FR), Univ.Catania (It), INL (FR), HORIBA (FR)*

*Techniques:* *CBVD, Raman, HR-XRD, SEM, rf-GDOES, AFM, ellipsometry, M-Line.*

*Materials:* *$LiNbO_3$*

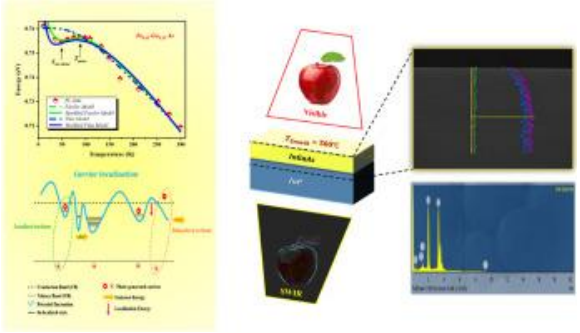

### *Abstract*

*In this work, we demonstrated the potential of rapid optimization of high quality (006) $LiNbO_3$ deposited thin film on c-sapphire by combinatorial Chemical Beam Vapour Deposition. In the best identified chemical precursor ratio, films demonstrated a chemical composition close to stoichiometry, and revealed excellent epitaxial quality (mosaïcity of 0.04° for 350 nm thick films), despite the presence of twins, and optical properties compatible with light guiding, with an index of refraction similar to bulk crystal one.*


*OPERA Work Group*

*WG3*

## Experimental insights toward carrier localization in in-rich InGaAs/InP as candidate for SWIR detection: Microstructural analysis combined with optical investigation



*Reference:* *Materials Science in Semiconductor Processing, 153, 107149. (2023); doi; 10.1016/j.mssp.2022.107149*

*Authors:* *Arbia, M. B., Demir, I., Kaur, N., Saidi, F., Zappa, D., Comini, E., Altuntaş, I., and Maaref, H.*

*Laboratories:* *Laboratoire de Micro-optoélectronique et Nanostructures (Tn), and The Nanophotonics Research and Application Center at Sivas Cumhuriyet University (CUNAM) (Tr)*

*Techniques:* *MOVPE, XRD, PL, UV- VIS Spectrophotometer, SEM-EDX, Raman, AFM*

*Materials:* *InGaAs/InP*

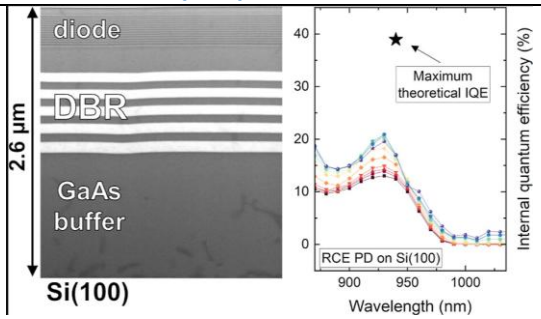
*Abstract*

*Hyperspectral imaging has been flourished thanks to the huge investigation of the infrared spectrum from NIR to LWIR bands. The ternary InGaAs has been investigated herein in the context of studying the structural dependences of localization phenomenon by X-ray diffraction (XRD), scanning electron microscopy-energy dispersive X-ray (SEM-EDX), Raman, ultraviolet–visible (UV–vis), and photoluminescence (PL) techniques. Using metal-organic vapor phase epitaxy (MOVPE), we succeed to grow the InGaAs directly on InP substrate at 560 °C as an active layer with indium concentration exceeding the "golden" value (53%) to enlarge its cutoff absorption wavelength. X-ray diffraction proved a good crystallinity of the heterostructure with a sharp peak related to the thick substrate and another peak attributed to the thin layer of InGaAs. Moreover, an interfacial layer appeared at the logarithmic scale of XRD patterns and was confirmed by Raman analysis. The SEM-EDX revealed an average indium concentration (62%), almost the growth concentration. However, a cross-section compositional profile over the heterostructure showed an inhomogeneous distribution of the indium. This is predictable from the composition fluctuation in the indium-containing alloys and the volatility (surface segregation) of As (In). On the other side, the optical investigation of InGaAs demonstrated an anomalous behavior of luminescence versus temperature, manifested by the S-shape feature. This trend stems from the potential fluctuation induced by the non-uniform distribution of indium. A numerical simulation was developed based on the localized state ensemble (LSE) model to well-reproduce this anomaly by giving the best fitting parameters and comparing them with those calculated using the semi-empirical models (Viña and Pässler). The results reported here will help in optimizing the epitaxy design of future InGaAs/InP and further studying its surface morphology and device performance.*

*OPERA Work Group*

*WG2*

## InGaAs/GaAsP Superlattice Resonant Cavity-Enhanced Photodetector Fabricated on a Nominal Si(001) Substrate for Near- and Short-Wavelength Infrared Applications





### Abstract

*The III–V materials offer superior optoelectronic performance that makes them an attractive choice for integration into cheap and ubiquitous Si-based technologies, contingent upon addressing the consequences of the prohibitively large lattice constant mismatch between the two material systems. We present a near-infrared (NIR) resonant cavity-enhanced photodetector (RCE PD) monolithically integrated onto a nominal Si(001) substrate and incorporating a thin InGaAs/GaAsP strained-layer superlattice acting as the absorber, as well as five repetitions of GaAs/AlGaAs distributed Bragg reflectors providing resonant enhancement. The photodetector was metal–organic chemical vapor deposition-grown onto the Si(001) substrate using a buffer incorporating simultaneously a GaAs bulk layer and the distributed Bragg reflector (DBR) stack, a two-step growth temperature sequence, and an optimized thermal cycle annealing process, with a total structure thickness of 2.6 µm. The device demonstrates 13–21% internal quantum efficiency against the theoretical maximum of 39%, a result that is easily extendable via the addition of DBR pairs or other reflectors. Thanks to the thin absorber design inherent to the RCE PD architecture, the dark current density of the Si-based device is reduced to the same order of magnitude ($\sim 10^{-8}$ A cm$^{-2}$) as an identical structure grown on a lattice-matched GaAs substrate. In general, the promising structural and optoelectronic results for this device represent a viable track to direct monolithic integration of III–V materials onto Si wafers, while the tunability of the InGaAs/GaAsP superlattice system opens up the potential for extended NIR and short-wavelength infrared coverage.*



*Reference:* *ACS Photonics 2023, 10, 9, 3266–3274; DOI:* 10.1063/5.0219507



*Authors:* *V. Letka, M. Martin, N. Massara, C. Leroux, R. Templier, C. Licitra, J. Richy, and T. Baron*


*Laboratories:* *LTM (Fr), LETI (Fr)*

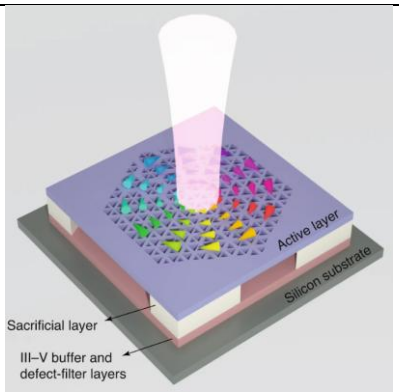
*Techniques:* *MOCVD, STEM, PL, AFM, XRD, Nextnano*

*Materials:* *III-V/Si(001)*

### OPERA Work Group

*WG3*

## Room-temperature continuous-wave topological Dirac-vortex microcavity lasers on silicon





### Abstract

*Robust laser sources are a fundamental building block for contemporary information technologies. Originating from condensed-matter physics, the concept of topology has recently entered the realm of optics, offering fundamentally new design principles for lasers with enhanced robustness. In analogy to the well-known Majorana fermions in topological superconductors, Dirac-vortex states have recently been investigated in passive photonic systems and are now considered as a promising candidate for robust lasers. Here, we experimentally realize the topological Dirac-vortex microcavity lasers in InAs/InGaAs quantum-dot materials monolithically grown on a silicon substrate. We observe room-temperature continuous-wave linearly polarized vertical laser emission at a telecom wavelength. We confirm that the wavelength of the Dirac-vortex laser is topologically robust against variations in the cavity size, and its free spectral range defies the universal inverse scaling law with the cavity size. These lasers will play an important role in CMOS-compatible photonic and optoelectronic systems on a chip.*



*Reference:* *Light Sci. Appl.* ***12****(1), 255 (2023)*
DOI : 10.1038/s41377-023-01290-4



*Authors:* J. Ma, T. Zhou, M. Tang, H. Li, Z. Zhang, X. Xi, M. Martin, T. Baron, H. Liu, Z. Zhang, S. Chen, and X. Sun


*Laboratories:* *The Chinese University of Hong Kong(CN), LTM(Fr), UCL(UK).*

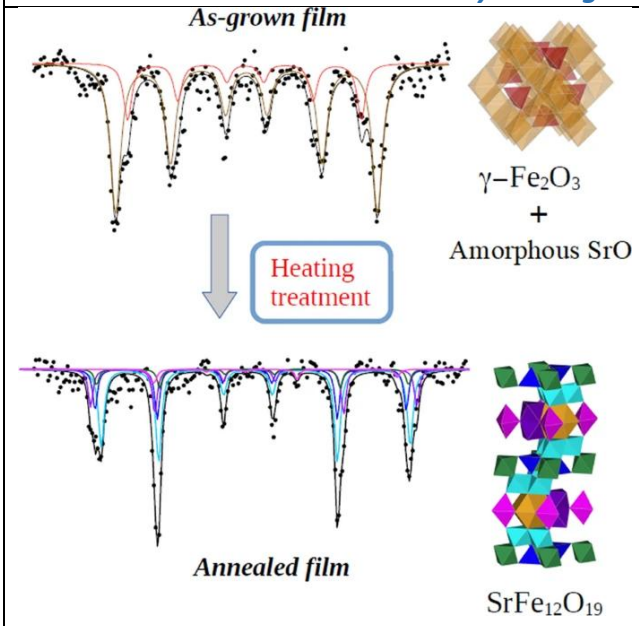
*Techniques:* *MOCVD, MBE, µPL, COMSOL/Lumerical*

*Materials:* *III-V/Si(001)*

### OPERA Work Group

*WG2 & WG3*

## *Effect of annealing in the formation of well crystallized and textured SrFe12O19 films grown by RF magnetron sputtering*




*Reference:* *Journal of Materials Research 38, 1119 (2023), DOI: 10.1557/s43578-022-00822-9*

*Authors:* *G.D. Soria, A. Serrano, J.E. Prieto, A. Quesada, G. Gorni, J. de la Figuera, J.F. Marco*

*Laboratories:* *Instituto de Química Física Blas Cabrera (ES), Instituto de Cerámica y Vidrio (ES), Universidad Complutense de Madrid (ES)*

*Techniques:* *Magnetron sputtering*

*Materials:* *Oxides*

*Abstract*

*In this work, We have studied the influence of the annealing treatment on the crystalline growth of SrFe12O19 previously deposited on Si (100) substrates using radio frequency (RF) magnetron sputtering. For this goal, two grown films, with and without ex situ heating step, have been analyzed and compared to determine the differences in their structural, compositional, and magnetic properties. The results obtained by the different analysis techniques, in particular Mössbauer spectroscopy together with EXAFS and XANES data, suggest that the as-grown film is composed of nanocrystalline maghemite nanoparticles and amorphous strontium oxide. Specifically, Mössbauer spectroscopy results pointed out the presence of Fe3+ cations occupying octahedral and tetrahedral sites with hyperfine magnetic fields 49.3 T and 44.2 T, respectively, characteristic of a spinel-related structure. A strontium hexaferrite canonical structure with a c-axis orientation in the sample plane was found for the annealed film.*

*OPERA Work Group*

*WG2*