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

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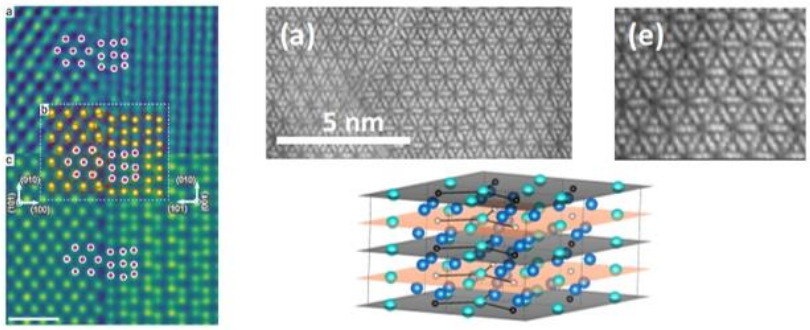
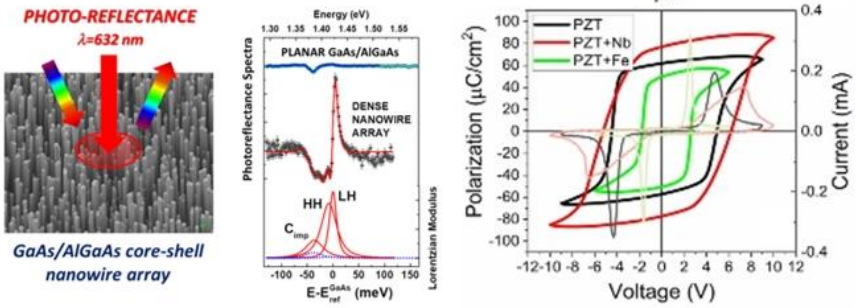
COST Action CA20116

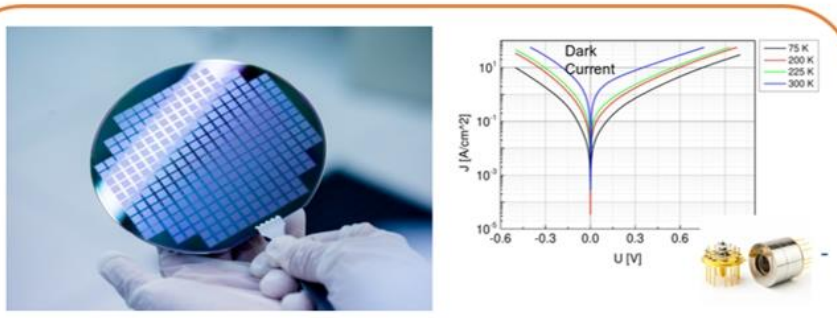
Highlights 2022



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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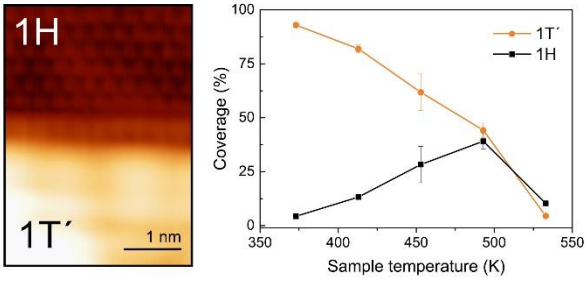
I- Fundamental research – New Materials (WG1)

Phase control and lateral heterostructures of $MoTe_2$ epitaxially grown on graphene/Ir(111)



Reference: *Nanoscale 14, 10880-10888(2022).*

Authors: *J. Ripoll-Sau, F. Calleja, P. Casado Aguilar, I. M. Ibarburu, A. L. Vázquez de Parga, R. Miranda and M. Garnica*

Laboratories: *IMDEA Nanoscience and Universidad Autónoma de Madrid* ***(Es)***

Techniques: *MBE, STM*

Materials: *$MoTe_2$, graphene/Ir(111)*

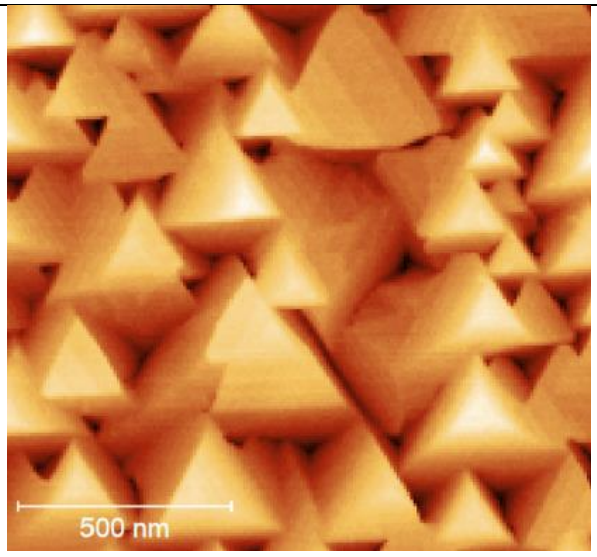
Abstract

Engineering the growth of the different phases of two-dimensional transition metal dichalcogenides (2D-TMDs) is a promising way to exploit their potential since the phase determines their physical and chemical properties. Here, we report on the epitaxial growth of monolayer $MoTe_2$ on graphene on an Ir(111) substrate. Scanning tunneling microscopy and spectroscopy provide insights into the structural and electronic properties of the different polymorphic phases, which remain decoupled from the substrate due to the weak interaction with graphene. In addition, we demonstrate a great control of the relative coverage of the relevant 1T' and 1H $MoTe_2$ phases by varying the substrate temperature during the growth. In particular, we obtain large areas of the 1T' phase exclusively or the coexistence of both phases with different ratios.

OPERA Work Group

WG1

Structure of Strained Low-Dimensional Sb by In Situ Surface X-Ray Diffraction



Reference: *physica status solidi (b) 259(4); doi: 10.1002/pssb.202100432*

Authors: *P. Mousley, C. Burrows, C. Nicklin, G.R. Bell*

Laboratories: *University of Warwick, Diamond Light Source* ***(GB)***

Techniques: *MBE, surface X-ray diffraction (SXRD), RHEED, XPS, AFM*

Materials: *Sb, InAs*

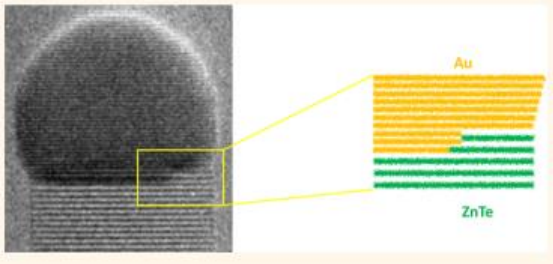
Abstract

It is possible to perform surface X-ray diffraction (SXRD) at several synchrotron radiation beamlines around the world. At Diamond Light Source, beamline I07 also allows the co-deposition of small thicknesses of most materials in the SXRD scattering chamber itself so that simple MBE growth can be done. For MBE growers, SXRD can be seen as a sort of "super RHEED" allowing detailed and quantitative structural characterization on pristine films and surfaces in ultra-high vacuum. In this work we have grown ultra-thin films of antimony, Sb(0001), on nearly lattice-matched InAs(111)B substrates. The films studied in detail are 4 and 19 Sb atomic bilayers thick. They are both fully strained in-plane, and show complex out-of-plane relaxations. The abruptness of the interface has been quantified, with intermixing of Sb and As over 2 atomic layers. A small fraction of rotational twin domains are identified, and there is neither interfacial nor surface reconstruction. For ultra-thin Sb films we saw no evidence of antimonene. Thicker Sb films begin to form shallow pyramidal facet structures, as shown in the AFM image.

OPERA Work Group

WG1

Regulated dynamics with two monolayer steps in vapor-solid-solid growth of nanowires



Reference: ACS Nano 16, 4397-4407 (2022); DOI: 10.1021/acsnano.1c10666

Authors: E. Bellet-Amalric, F. Panciera, G. Patriarche, L. Travers, M. den Hertog, J.-C. Harmand, F. Glas, J. Cibert

Laboratories: CEA/IRIG **(Fr)**, C2N **(Fr)**, Institut Néel **(Fr)**

Techniques: MBE, in situ TEM, growth modelling

Materials: ZnTe, CdTe nanowires

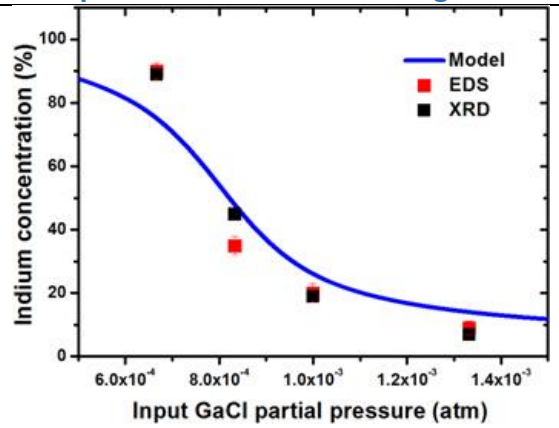
Abstract

The growth of ZnTe nanowires and ZnTe-CdTe nanowire heterostructures is studied by in situ transmission electron microscopy. We describe the shape and the change of shape of the solid gold nanoparticle during vapor-solid-solid growth. We show the balance between one monolayer and two monolayer steps, which characterizes the vapor-liquid-solid and vapor-solid-solid growth modes of ZnTe. We discuss the likely role of the mismatch strain and lattice coincidence between gold and ZnTe on the predominance of two monolayer steps during vapor-solid-solid growth and on the subsequent self-regulation of the step dynamics. Finally, the formation of an interface between CdTe and ZnTe is described

OPERA Work Group

WG1

Compositional control of homogeneous InGaN nanowires with the In content up to 90%



Reference: Mohammed Zeghouane et al 2019 Nanotechnology 30 044001. Doi:10.1088/1361-6528/aaec39

Authors: M. Zeghouane, G. Avit, Y. André, C. Bougerol, Y. Robin, P. Ferret, D. Castelluci, E. Gil, V. G Dubrovskii, H. Amano, A. Trassoudaine

Laboratories: UCA Clermont-Ferrand **(Fr)**, ITMO University **(Ru)**, Université Grenoble-Alpes, CNRS-Institut Néel **(Fr)**, IMSS Nagoya **(Jp)**, CEA-DRT LETI/DTS, Grenoble **(Fr)**

Techniques: HVPE

Materials: InGaN

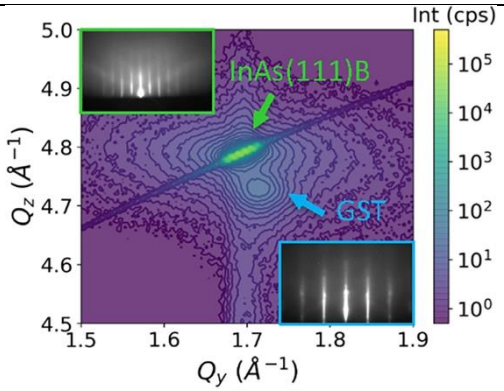
Abstract

Homogenous InGaN nanowires with a controlled indium composition up to 90% are grown on GaN/c-Al2O3 templates by catalyst-free hydride vapor phase epitaxy using InCl3 and GaCl as group III element precursors. The influence of the partial pressures on the growth rate and composition of InGaN nanowires is investigated. It is shown how the InN mole fraction in nanowires can be finely tuned by changing the vapor phase composition. Thermodynamic calculations are presented that take into account different interconnected reactions in the vapor phase and show a good agreement with the compositional data. Energy dispersive x-ray spectroscopy profiles performed on single nanowires show a homogenous indium composition along the entire nanowire length. X-ray diffraction measurements performed on nanowires arrays confirm these data. High-resolution transmission electron microscopy analysis shows the wurtzite crystal structure with a reduced defect density for InGaN nanowires with the highest indium content.

OPERA Work Group

WG1

Hints for a General Understanding of the Epitaxial Rules for van der Waals Epitaxy from Ge-Sb-Te Alloys



Reference: *Adv. Mater. Interfaces 9 2101556 (2022); doi: 10.1002/admi.202101556*

Authors: *F. Arciprete, J. E. Boschker, S. Cecchi, E. Zallo, V. Bragaglia, and R. Calarco*

Laboratories: *Un. of Rome Tor Vergata **(It)**, Paul-Drude Institut **(De)***

Techniques: *MBE, XRD, Raman*

Materials: *Ge-Sb-Te alloys, InAs*

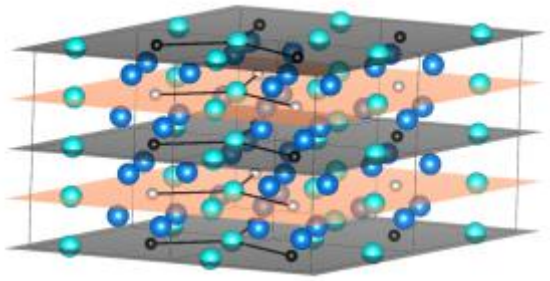
Abstract

In this study, a generalized guideline is identified to predict the interaction between two-dimensional (2D) layered materials and substrate surfaces. Additionally, the van der Waals (vdW) heterostructures commensurability, the phase formation and the strain relaxation are identified during interface growth. To achieve such a general overview, the case of Ge-Sb-Te (GST) alloys on InAs(111) is studied. In this system, low-lattice mismatch conditions are fulfilled to avoid relaxation due to formation of misfit dislocations and allow to correctly identify vdW epitaxy. At the same time, the substrate can be efficiently prepared into self- and un-passivated surfaces to clarify the role of the surface interaction. Furthermore, the GST epilayer exhibits two different highly ordered 2D structures and a three-dimensional disordered structure, allowing to directly infer the nature of the epitaxy. This study opens the way for the design and mastering of vdW epitaxial growth of 2D heterostructures as well as hybrid 2D and non-layered materials.

OPERA Work Group

WG1

Highly ordered carbon penetration into the $Mn_5Ge_3C_x$ lattice: A superstructure in $Mn_5Ge_3C_{0.5}$ inferred from a ^{55}Mn NMR study



Reference: *Physical Review B 2022, 105, 094405; DOI: 10.1103/PhysRevB.105.094405*

Authors: *R. Kalvig, E. Jedryka, M. Wojcik, M. Petit, L. Michez*

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

Techniques: *NMR, MBE*

Materials: *MBE grown Mn_5Ge_3 thin films doped with carbon*

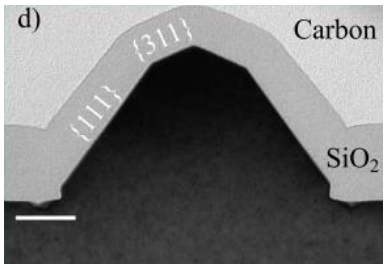
Abstract

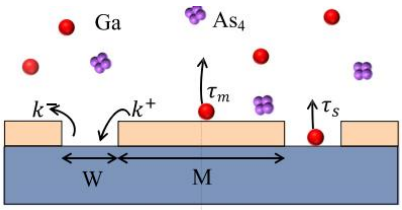
Our extensive ^{55}Mn NMR study performed on a series of $Mn_5Ge_3C_x$ ($0<x<0.85$) films with a good epitaxial quality provides strong evidence for a highly correlated carbon penetration into the Mn_5Ge_3 structure, setting the limit for the carbon uptake at $x = 0.5$. A superstructure, consisting in a selective fulfillment of the available lattice voids by carbon, has been postulated for $x = 0.5$, based on the short range order directly observed in the NMR experiments. Such a nanolaminated structure, where only every second atomic plane hosts carbon atoms, is likely to display new, interesting phenomena, opening the way for further exploration of spintronic effects in this system.

OPERA Work Group

WG1

Selective Area Epitaxy of GaAs: The unintuitive role of slit size and pitch





Abstract

Selective area epitaxy (SAE) provides the path for scalable fabrication of semiconductor nanostructures in a device-compatible configuration. In the current paradigm, SAE is understood as localized epitaxy, and is modelled by combining planar and self-assembled nanowire growth mechanisms. Here we use GaAs SAE as a model system to provide a different perspective. First, we provide evidence of the significant impact of the annealing stage in the calculation of the growth rates. Then, by elucidating the effect of geometrical constraints on the growth of the semiconductor crystal, we demonstrate the role of adatom desorption and resorption beyond the direct-impingement and diffusion-limited regime. Our theoretical model explains the effect of these constraints on the growth, and in particular why the SAE growth rate is highly sensitive to the pattern geometry. Finally, the disagreement of the model at the largest pitch points to nonnegligible multiple adatom recycling between patterned features. Overall, our findings point out the importance of considering adatom diffusion, adsorption and desorption dynamics in designing the SAE pattern to create pre-determined nanoscale structures across a wafer. These results are fundamental for the SAE process to become viable in the semiconductor industry.

Reference: *Nanotechnology 33, 485604 (2022). DOI 10.1088/1361-6528/ac88d9*

Authors: *D. Dede, F. Glas, V. Piazza, N. Morgan, M. Friedl, L. Güniat, E. N. Dayi, A. Balgarkashi, V. G. Dubrovskii, A. Fontcuberta i Morral*

Laboratories: *EPFL Lausanne **(Ch)**, C2N **(Fr)**, St Petersburg State University **(Ru)***

Techniques: *MBE, growth modelling*

Materials: *GaAs nanomembranes*

OPERA Work Group

WG1

Interfacial profile of axial nanowire heterostructures in the nucleation limited regime

CrystEngComm

Abstract

Heterostructured nanowires exhibit unique physical and electronic properties and are most commonly grown by the vapor–liquid–solid mechanism. Some of these properties are related to the interfacial abruptness of the heterointerface which makes its understanding and control particularly important for further development. In this regard, we present a model based on mass balance of atoms in the catalyst droplet where the atoms incorporate into the solid in the nucleation-limited regime. We explain how and why the decrease of growth temperature and increase of the flux of an element which forms a heterostructure leads to an improvement in the interface abruptness. Our model demonstrates that a sharp heterointerface can be obtained if one uses a high concentration of the foreign catalyst rather than selfcatalyzed growth, which can be explained by a reduced reservoir effect. For the examples of InAs/GaAs and GaAs/AlAs heterostructures, we compare the compositional profiles for the two different heterointerface directions.

Reference: *CrystEngComm 24, 8052 (2022); doi: 10.1039/d2ce01337a.*

Authors: *E. D. Leshchenko and J. Johansson*

Laboratories: *NanoLund, Lund University **(Se)***

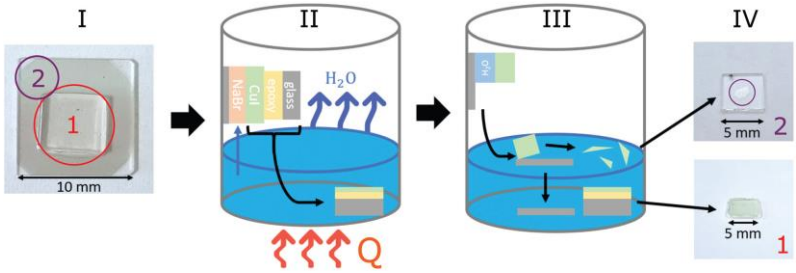
Techniques: *Nucleation and mass-transport modeling*

Materials: *Au catalyzed InAs/GaAs and GaAs/AlAs semiconductor heterostructures*

OPERA Work Group

WG1

Epitaxial lift-off of single crystalline CuI thin films



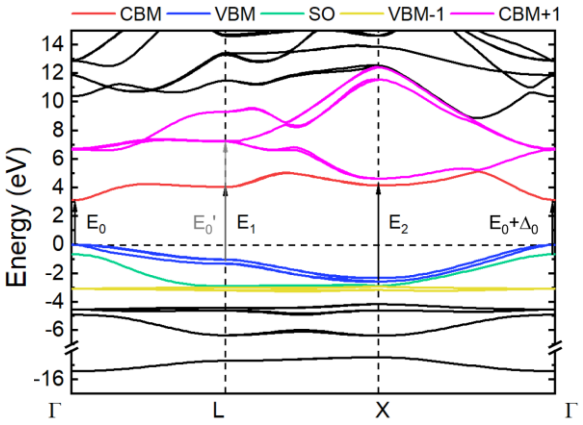
Reference: *J. Mater. Chem. C, 2022, 10, 4124;*
DOI: https://doi.org/10.1039/d2tc00083k
Authors: *P. Storm, S. Selle, H. von Wenckstern, M. Grundmann, and M. Lorenz*
Laboratories: *Univ. Leipzig **(De)**, FhG IMWS Halle **(De)***
Techniques: *PLD, lift-off, XRD, SEM, AFM*
Materials: *CuI, NaBr, SrF_2*

Abstract

Thin films of the transparent, p-type semiconductor copper iodide (CuI) were grown by pulsed laser deposition on SrF_2(111) with water soluble sodium bromide (NaBr) sacrificial layers. The resulting epitaxial CuI thin films are single crystalline and offer reduced surface roughness compared to epitaxial CuI grown with rotational domains on other templates. The CuI thin films were transferred onto glass using epoxy/glue and dissolution of the NaBr in a water vapor atmosphere.

OPERA Work Group
WG1

Dielectric function of $CuBr_xI_{1-x}$ alloy thin films



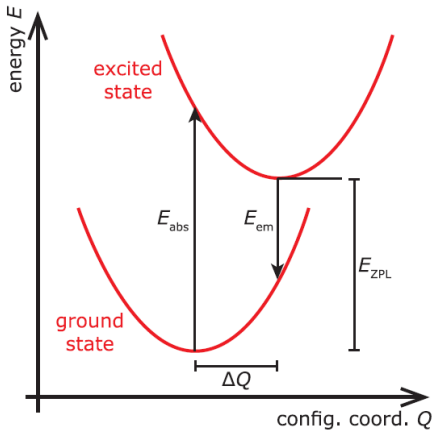
Reference: *Physical Review Materials 2022, 6, 124601;*
DOI: https://doi.org/10.1103/PhysRevMaterials.6.124601
Authors: *M. Seifert, E. Krüger, M. S. Bar, S. Merker, H. von Wenckstern, H. Krautscheid, M. Grundmann, C. Sturm, and S. Botti*
Laboratories: *F.-S.-Univ. Jena **(De)**, Univ. Leipzig **(De)***
Techniques: *PLD, spectroscopic ellipsometry, XRD, DFT*
Materials: *$CuBr_xI_{1-x}$, Al_2O_3*

Abstract

We study the dielectric function of $CuBr_xI_{1-x}$ thin film alloys using spectroscopic ellipsometry in the spectral range between 0.7 eV and 6.4 eV, in combination with first-principles calculations based on density functional theory. Through the comparison of theory and experiment, we attribute features in the dielectric function to electronic transitions at specific k-points in the Brillouin zone. The observed band gap bowing as a function of alloy composition is discussed in terms of different physical and chemical contributions. The band splitting at the top of the valence band due to spin-orbit coupling is found to decrease with increasing Br-concentration, from a value of 660 meV for CuI to 150 meV for CuBr. This result can be understood considering the contribution of copper d orbitals to the valence band maximum as a function of the alloy composition.

OPERA Work Group
WG1

Light Absorption and Emission by Defects in Doped Nickel Oxide



Reference: *Adv. Photonics Res. 2022, 3, 2200138;*
DOI: https://doi.org/10.1002/adpr.202200138

Authors: *R. Karsthof, Y. K. Frodason, A. Galeckas, P. M. Weiser, V. Zviagin, and M. Grundmann*

Laboratories: *Univ. Oslo **(No)**, Univ. Leipzig **(De)***

Techniques: *PLD, DC-sputtering, XRD, Hall, UV/VIS/NIR, DUV, spectroscopic ellipsometry, PL, DFT*

Materials: *NiO*

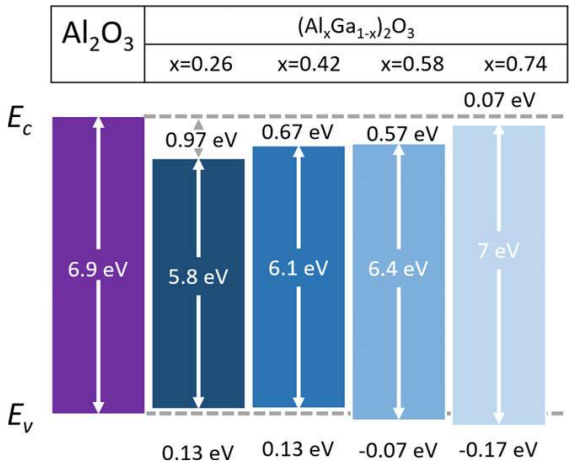
Abstract

Nickel oxide is a versatile p-type semiconducting oxide with many applications in optoelectronic devices, but high doping concentrations are often required to achieve necessary electrical conductivity. In contrast to many other transparent oxide semiconductors, even moderate doping levels in NiO can lead to significant optical absorption in the visible spectral range, limiting the application range of the material. This correlation has been reported extensively in the literature, but its origin has been unknown until now. This work combines experimental data on optical properties from a variety of NiO samples with results from hybrid density functional theory calculations. It shows that strong electron–phonon interaction leads to a significant blueshift (0.6–1 eV) of electronic transitions from the valence band maximum to defect states by light absorption with respect to the thermodynamic charge transition levels. This essentially renders NiO a narrow-gap semiconductor by defect band formation already at moderate doping levels, with strong light absorption for photon energies of approximately 1 eV. The calculations are also shown to be fully consistent with experimental data on defect-related light emission in NiO.

OPERA Work Group

WG1

Band Alignment of Al_2O_3 on α-$(Al_xGa_{1-x})_2O_3$



Reference: *ECS J. Solid State Sci. Technol. 2022, 11, 025006;*
DOI: https://doi.org/10.1149/2162-8777/ac546f

Authors: *X. Xia, N. S. Al-Mamun, C. Fares, A. Haque, F. Ren, A. Hassa, H. von Wenckstern, M. Grundmann, and S. J. Pearton*

Laboratories: *Univ. Florida **(US)**, Penn. State Univ. **(US)**, Univ. Leipzig **(De)***

Techniques: *PLD, ALD, EDAX, XRD, TEM, XPS, REELS*

Materials: *α-$(Al_xGa_{1-x})_2O_3$, Al_2O_3*

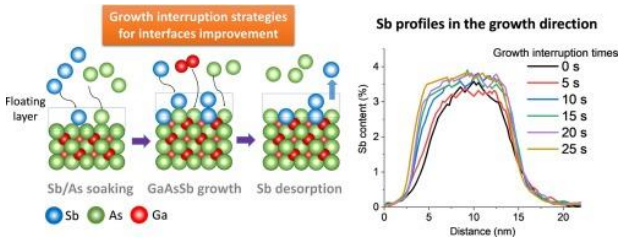
Abstract

X Ray Photoelectron Spectroscopy was used to measure valence band offsets for Al_2O_3 deposited by Atomic Layer Deposition on α-$(Al_xGa_{1-x})_2O_3$ alloys over a wide range of Al contents, x, from 0.26–0.74, corresponding to a bandgap range from 5.8–7 eV. These alloys were grown by Pulsed Laser Deposition. The band alignments were type I (nested) at x <0.5, with valence band offsets 0.13 eV for x = 0.26 and x = 0.46. At higher Al contents, the band alignment was a staggered alignment, with valence band offsets of − 0.07 eV for x = 0.58 and −0.17 for x = 0.74, i.e. negative valence band offsets in both cases. The conduction band offsets are also small at these high Al contents, being only 0.07 eV at x = 0.74. The wide bandgap of the α-$(Al_xGa_{1-x})_2O_3$ alloys makes it difficult to find dielectrics with nested band alignments over the entire composition range.

OPERA Work Group

WG1

Growth interruption strategies for interface optimization in GaAsSb/GaAsN type-II superlattices



Abstract

Recently, GaAsSb/GaAsN type II short-period superlattices (SLs) have been proposed as suitable structures to be implemented in the optimal design of monolithic multi-junction solar cells. However, due to strong surface Sb segregation, experimental Sb composition profiles differ greatly from the nominal square-wave design. In this work, the improvement of the interface quality of these SLs in terms of compositional abruptness and surface roughness has been evaluated by implementing different growth interruption times under Sb4/As4 (soaking) and As4 (desorption) overpressure conditions before and after the growth of GaAsSb layers, respectively. The combined effects of both processes enhance Sb distribution, achieving squarer compositional profiles with reduced surface roughness interfaces. It has been found that the improvement in compositional abruptness is quantitatively much higher at the lower interface, during soaking, than at the upper interface during desorption. Conversely, a larger decrease in surface roughness is achieved at the upper interface than at the lower interface. Fitting of the Sb segregation profiles using the 3-layer kinetic fluid model has shown that the increase in Sb incorporation rate is due to the decrease in segregation energy, presumably to changes in the surface reconstruction of the floating layer at the surface.

Reference:
Applied Surface Science 604 (2022) 154596; https://doi.org/10.1016/j.apsusc.2022.154596.

Authors:
V. Braza, T. Ben, S. Flores, D.F. Reyes, A. Gallego-Carro, L. Stanojevi`c, ˇZ. Gãcevi`c, N. Ruíz-Marín, J.M. Ulloa, D. Gonzalez.

Laboratories:
*University Research Institute on Electron Microscopy & Materials, IMEYMAT **(Es)**, University of Cádiz **(Es)**, Institute for Optoelectronic Systems and Microtechnology (ISOM), Madrid **(Es)***

Techniques:
MBE, STEM-EDX.

Materials:
GaAsSb-GaAs superlattices on GaAs substrate.

OPERA Work Group
WG1

Tailoring of AlAs/InAs/GaAs QDs Nanostructures via Capping Growth Rate

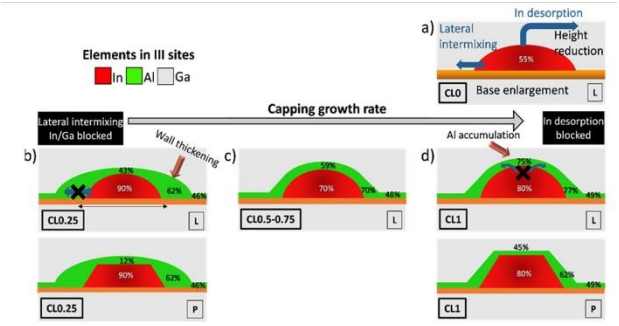


Figure. Schematic representation of the CGR effects in the GaAs/InAs/AlAs QD system QD capped with GaAs (CL0), (b) covered by AlAs at 0.25 ML/s (CL0.25), (c) 0.5–0.75 ML/1 ML/s (CL1). "L" and "P" at the bottom right in each picture designate the lens and pyramidal geometries. Average compositions for the QDs and the CL

Abstract

The use of thin AlA capping layers (CLs) on InAs quantum dots (QDs) has recently received considerable attention due to improved photovoltaic performance in QD solar cells. However, there is little data on the structural changes that occur during capping and their relation to different growth conditions. In this work, we studied the effect of AlA capping growth rate (CGR) on the structural features of InAs QDs in terms of shape, size, density, and average content. As will be shown, there are notable differences in the characteristics of the QDs upon changing CGR. The Al distribution analysis in the CL around the QDs was revealed to be the key. On the one hand, for the lowest CGR, Al has a homogeneous distribution over the entire surface, but there is a large thickening of the CL on the sides of the QD. As a result, the QDs are lower, lenticular in shape, but richer in In. On the other hand, for the higher CGRs, Al accumulates preferentially around the QD but with a more uniform thickness, resulting in taller QDs, which progressively adopt a truncated pyramidal shape. Surprisingly, intermediate CGRs do not improve either of these behaviors, resulting in less enriched QDs.

Reference:
Nanomaterials 2022, 12, 2504. https://doi.org/10.3390/nano12142504

Authors:
N. Ruiz , D. Fernandez, E. Luna , L. Stanojevi`c , T. Ben , S. Flores, V. Braza , A. Gallego-Carro , G. Bárcena-González , A. Yañez , J. M. Ulloa and D. González

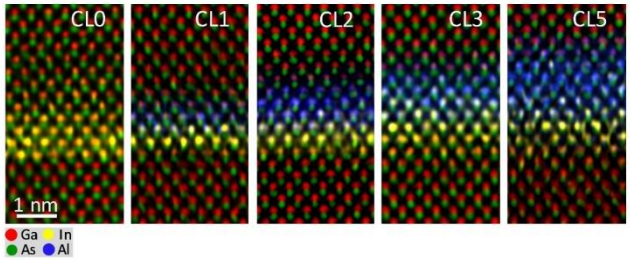
Laboratories:
*University Research Institute on Electron Microscopy & Materials, IMEYMAT **(Es)**, University of Cádiz **(Es)**, Institute for Optoelectronic Systems and Microtechnology (ISOM), Madrid **(Es)***

Techniques:
MBE, STEM-EDX, EELS-STEM

Materials:
AlAs capped-InAs quantum dots on GaAs substrate.

OPERA Work Group
WG1

Suppressing the Effect of theWetting Layer through AlAs Capping in InAs/GaAs QD Structures for Solar Cells Applications



Reference: *Nanomaterials 2022, 12, 1368. https://doi.org/10.3390/nano12081368*

Authors: *N. Ruiz , D. Fernández , L. Stanojevi´c, T. Ben , S. Flores, V. Braza, A. Gallego Carro, E. Luna,, J. M. Ulloa and D. González*

Laboratories: *University Research Institute on Electron Microscopy & Materials, IMEYMAT **(Es)**, University of Cádiz **(Es)**, Institute for Optoelectronic Systems and Microtechnology (ISOM), Madrid **(Es)***

Techniques: *MBE, HR-STEM-EDX, EELS-STEM*

Materials: *AlAs capped-InAs quantum dots on GaAs substrate.*

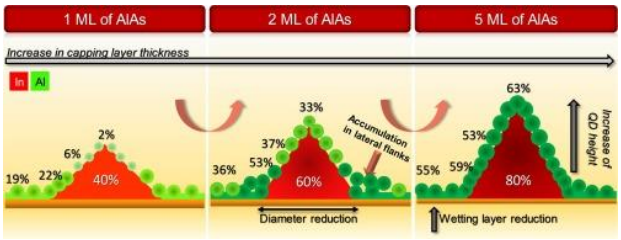
Abstract

Recently, thin AlAs capping layers (CLs) on InAs quantum dot solar cells (QDSCs) have been shown to yield better photovoltaic efficiency compared to traditional QDSCs. Although it has been proposed that this improvement is due to the suppression of the capture of photogenerated carriers through the wetting layer (WL) states by a de-wetting process, the mechanisms that operate during this process are not clear. In this work, a structural analysis of the WL characteristics in the AlAs/InAs QD system with different CL-thickness has been made by scanning transmission electron microscopy techniques. First, an exponential decline of the amount of InAs in the WL with the CL thickness increase has been found, far from a complete elimination of the WL. Instead, this reduction is linked to a higher shield effect against QD decomposition. Second, there is no compositional separation between the WL and CL, but rather single layer with a variable content of InAlGaAs. Both effects, the high intermixing and WL reduction cause a drastic change in electronic levels, with the CL making up of 1–2 monolayers being the most effective configuration to reduce the radiative-recombination and minimize the potential barriers for carrier transport.

OPERA Work Group

WG1

Effect of the AlAs capping layer thickness on the structure of InAs/GaAs QD



Reference: *Applied Surface Science 573 (2022) 151572, https://doi.org/10.1016/j.apsusc.2021.151572*

Authors: *N. Ruiz , D. Fernández , L. Stanojevi´c, T. Ben , S. Flores, V. Braza, A. G. Carro, E. Luna, J.M. Ulloa and D. González*

Laboratories: *University Research Institute on Electron Microscopy & Materials, IMEYMAT **(Es)**, University of Cádiz **(Es)**, Institute for Optoelectronic Systems and Microtechnology (ISOM), Madrid **(Es)**.*

Techniques: *MBE, STEM-EDX, EELS-STEM*

Materials: *AlAs capped-InAs quantum dots on GaAs substrate.*

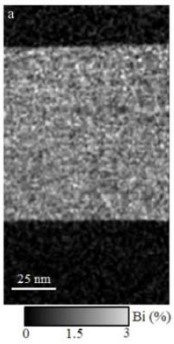
Abstract

Recently, very thin AlAs capping layers (CLs) have been proposed as a useful tool to increase the performance of InAs/GaAs quantum dot (QDs) devices. However, the structure of QDs after AlAs deposition remains poorly understood and the mechanisms to explain it are often contradictory. In this work, the structural and compositional changes of InAs QDs using different AlAs CL thicknesses have been studied by state-of-the-art STEM related techniques. First, the heights and In contents of InAs QDs progressively increase with the CL thickness, demonstrating that the AlAs capping produces a strong shielding effect against the decomposition of QDs. However, QD populations for CL thicknesses above 5 ML split into a bimodal distribution in which smaller lenticular QDs cohabit with bigger truncated pyramids. Second, the actual Al contents around the QDs are well below the nominal design, but increasing for thicker CLs. Its distribution is initially non-uniform, tending to accumulate on the flanks of the QDs to the detriment of the apex. Only for thicknesses above 2 ML the Al contents around the QDs start to be similar to those in the regions between the QDs, behaving as a continuous film without irregularities from 5 ML onwards.

OPERA Work Group

WG1

Effect of MBE growth conditions on GaAsBi photoluminescence lineshape and localised state filling



Reference: *Sci Rep 12, 797 (2022). https://doi.org/10.1038/s41598-021-04477-0*

Authors: *N.J. Bailey, T.B.O Rockett,. S. Flores, D.F. Reyes, J.P.R David,. R.D. Richards*

Laboratories: *University Research Institute on Electron Microscopy & Materials, IMEYMAT **(Es)**, University of Sheffield **(GB)**.*

Techniques: *MBE, STEM-EDX, XRD, RHEED, PL*

Materials: *Devices with $GaAs_xBi_{1-x}$ layers on GaAs substrate.*

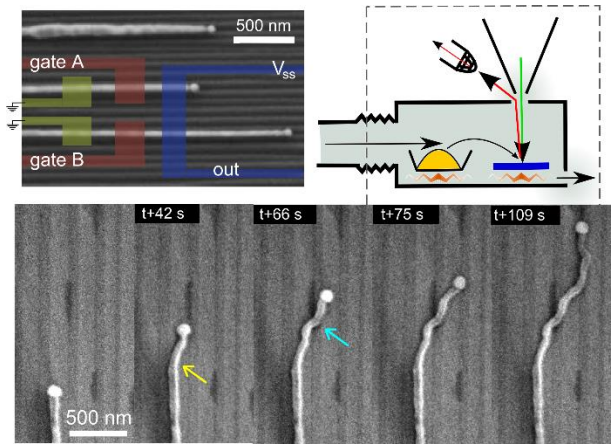
Abstract

A series of gallium arsenide bismide device layers covering a range of growth conditions are thoroughly probed by low-temperature, power-dependent photoluminescence measurements. The photoluminescence data is modelled using a localised state profile consisting of two Gaussians. Good agreement with the raw data is achieved for all layers whilst fixing the standard deviation values of the two Gaussians and constraining the band gap using X-ray diffraction data. The effects of growth temperature and bismuth beam equivalent pressure on the localised state distributions, and other model variables, are both shown to be linked to emission linewidth and device properties. It is concluded that bismuth rich surface conditions are preferable during growth in order to produce the narrowest emission linewidths with this material. These results also show how the growth mode of a gallium arsenide bismide layer can be inferred ex-situ from low-temperature photoluminescence measurements.

OPERA Work Group

WG1

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



Reference: *ACS Nano 16, 18757 (2022); DOI: 10.1021/acsnano.2c07480*

Authors: *A. Rothman, K. Bukvišová, N. R. Itzhak, I. Kaplan-Ashiri, A. E. Kossoy, X. Sui, L. Novák, T. Šikola, M. Kolíbal, E. Joselevich*

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

Techniques: *CVT, SEM*

Materials: *ZnSe nanowires*

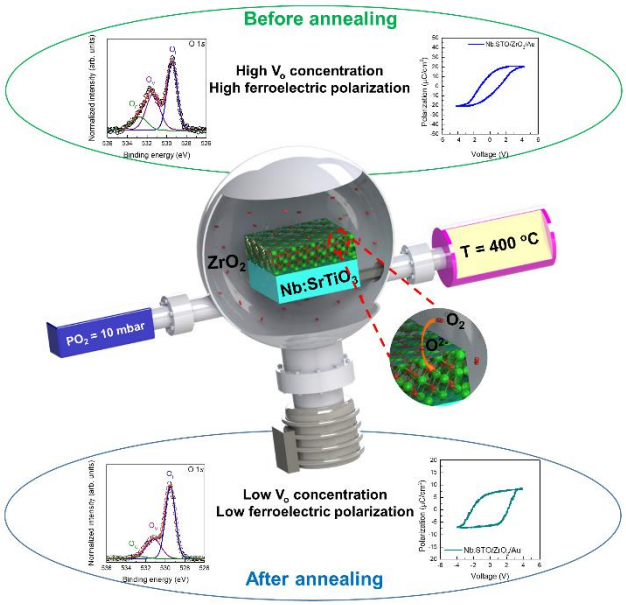
Abstract

Motivated by the concept of nanowire-based electronics, we observe how surface-guided nanowires grow in real time by in situ scanning electron microscopy (SEM). Movies of ZnSe surface-guided nanowires growing on periodically faceted substrates of annealed M-plane sapphire clearly show how the nanowires elongate along the substrate nanogrooves while pushing the catalytic Au nanodroplet forward at the tip of the nanowire. The movies reveal the timing between competing processes, such as planar vs nonplanar growth, catalyst-selective vapor–liquid–solid elongation vs nonselective vapor–solid thickening, and the effect of topographic discontinuities of the substrate on the growth direction, leading to the formation of kinks and loops. A decrease in precursor concentration as it is consumed after long reaction time causes the nanowires to shrink back instead of growing, thus indicating that the process is reversible and takes place near equilibrium. This real-time study of surface-guided growth, enabled by in situ SEM, enables a better understanding of the formation of nanostructures on surfaces.

OPERA Work Group

WG1

Ferroelectricity induced by oxygen vacancies in rhombohedral epitaxial ZrO_2 thin films



Reference: *Energy & Environmental Materials 2022* e12500
DOI: 10.1002/eem2.12500

Authors: *V. Lenzi, J. P. B. Silva, B. Šmíd, V. Matolín, C. M. Istrate, C. Ghica, J. L. MacManus-Driscoll, L. Marques*

Laboratories: *CF-UM-UP **(PT)**, UCAM **(GB)**, NIMP **(RO)**, CUNI **(CZ)***

Techniques: *IBD,XPS, HRTEM, P-E, I-V, DFT*

Materials: *ZrO_2/Nb:$SrTiO_3$*

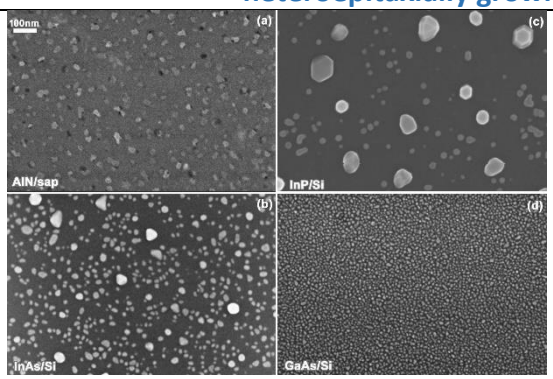
Abstract

Rhombohedral phase $Hf_xZr_{1-x}O_2$ (HZO, x from 0 to 1) films are promising for achieving robust ferroelectric polarisation without the need for an initial wake-up pre-cycling, as is normally the case for the more commonly studied orthorhombic phase. However, a large spontaneous polarisation observed in rhombohedral films is not fully understood, and there are also large discrepancies between experimental and theoretical predictions. In this work, in rhombohedral ZrO_2 thin films, we show that oxygen vacancies (V_O) are not only a key factor for stabilizing the phase, but they are also a source of ferroelectric polarisation in the films. This is shown experimentally through the investigation of the structural properties, chemical composition and the ferroelectric properties of the films before and after an annealing at moderate temperature (400 °C) in an oxygen environment to reduce the V_O concentration compared. The experimental work is supported by density functional theory (DFT) calculations which show that the rhombohedral phase is the most stable one in highly oxygen defective ZrO_2 films. The DFT calculations also show that V_O contribute to the ferroelectric polarisation. Our findings reveal the importance of Vo for stabilising rhombohedral ZrO_2 thin films with superior ferroelectric properties.

OPERA Work Group

WG1

On the origin of twist in 3D nucleation islands of tetrahedrally coordinated semiconductors heteroepitaxially grown along hexagonal orientations



Reference: *Journal of Applied Physics 132, 165102 (2022);*
DOI: 10.1063/5.0111558

Authors: *P. Vennéguès, L. Largeau, V. Brändli, B. Damilano, K. Tavernier, R. Bernard, A. Courville, S. Rennesson, F. Semond, G. Feuillet, and C. Cornet*

Laboratories: *CRHEA **(Fr)**, C2N **(Fr)**, Institut FOTON **(Fr)**, CEA-LETI **(Fr)**.*

Techniques: *MBE, SEM, TEM, XRD.*

Materials: *AlN/sapphire; InAs/Si(111); InP/Si(111); GaAs/Si(111)*

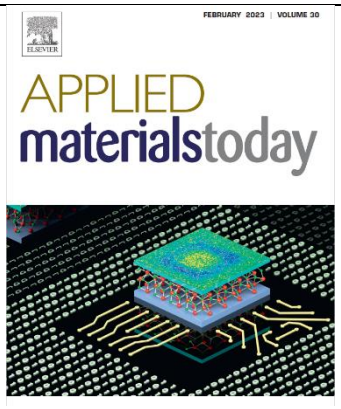
Abstract

In the first part of this paper, we present a model that explains and determines quantitatively the twists between nucleation islands in the case of a Volmer–Weber heteroepitaxial growth of tetrahedrally coordinated semiconductors along hexagonal orientations. These twists are caused by the network of the screw components of the 60° misfit dislocations. The orientations of the screw components are distributed randomly, and the maximum twist is obtained when all the screw components have the same orientation. The maximum twists are related to the density of misfit dislocations and, therefore, increase with the mismatch between the deposited materials and their substrate. In the second part of the paper, we study five systems having a large distribution of mismatches from 4% to 19%. For the four systems fulfilling the conditions necessary for the application of the model (plastic relaxation of grown islands), the measured maximum twists fit with the calculated values, thereby validating the model. The twists of nucleation islands are related to the mismatch and are, therefore, intrinsic to the material systems. The defects created at the coalescence of twisted islands determine the initial microstructure/defect distribution of the nucleation layer.

OPERA Work Group

WG1

Ferroelectricity and negative piezoelectric coefficient in orthorhombic phase pure ZrO_2 thin films



Reference: *Applied Materials Today 30, 2023, 101708*
DOI: 10.1016/j.apmt.2022.101708

Authors: *J. P.B. Silva, M. C. Istrate, M. Hellenbrand, A. Jan, M.n T. Becker, J. Symonowicz, F. G. Figueiras, V. Lenzi, M. O. Hill, C. Ghica, K. N. Romanyuk, M. J.M. Gomes, G. Di Martino, L. Marques, J. L. MacManus-Driscoll*

Laboratories: *CF-UM-UP **(Pt)**, UCAM **(GB)**, NIMP **(Ro)**, IFIMUP **(Pt)**, CICECO **(Pt)***

Techniques: *IBD, XRD, HRTEM, P-E, PFM, EBSD, DFT*

Materials: *ZrO_2/Nb:$SrTiO_3$*

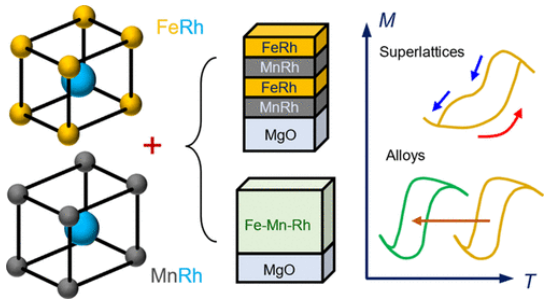
Abstract

A new approach for epitaxial stabilisation of ferroelectric orthorhombic (o-) ZrO_2 films with negative piezoelectric coefficient in ~8nm thick films grown by ion-beam sputtering is demonstrated. Films on (011)-Nb:$SrTiO_3$ gave the oriented o-phase, as confirmed by transmission electron microscopy and electron backscatter diffraction mapping, grazing incidence x-ray diffraction and Raman spectroscopy. Scanning probe microscopy techniques and macroscopic polarization-electric field hysteresis loops show ferroelectric behavior, with saturation polarization of ~14.3 μC/cm², remnant polarization of ~9.3 μC/cm² and coercive field ~1.2 MV/cm. In contrast to the o-films grown on (011)-Nb:$SrTiO_3$, films grown on (001)-Nb:$SrTiO_3$ showed mixed monoclinic (m-) and o-phases causing an inferior remnant polarization of ~4.8 μC/cm², over 50% lower than the one observed for the film grown on (011)-Nb:$SrTiO_3$. Density functional theory (DFT) calculations of the $SrTiO_3$/ZrO_2 interfaces support the experimental findings of a stable polar o-phase for growth on (011) Nb:$SrTiO_3$, and they also explain the negative piezoelectric coefficient.

OPERA Work Group

WG1

Controlling the metamagnetic phase transition in FeRh/MnRh superlattices and thin-film $Fe_{50-x}Mn_xRh_{50}$ alloys



Reference: *ACS Appl. Mater. Interfaces 14, 3568–3579 (2022); DOI: 10.1021/acsami.1c22460*

Authors: *M. Horký, J. A. Arregi, S. K. K. Patel, M. Staňo, R. Medapalli, O. Caha, L. Vojáček, M. Horák, V. Uhlíř, and E. E. Fullerton*

Laboratories: *CEITEC Brno University of Technology **(Cz)**, Masaryk University **(Cz)**, University of California San Diego **(US)***

Techniques: *Magnetron sputtering, x-ray diffraction, magnetometry*

Materials: *FeRh, MnRh*

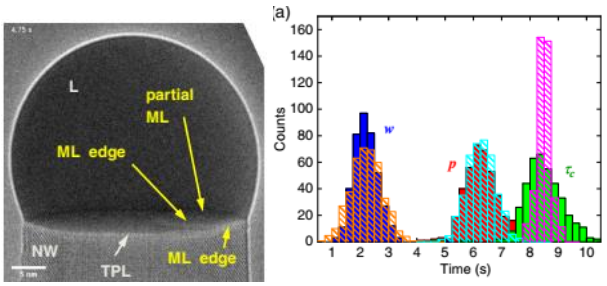
Abstract

Equiatomic and chemically ordered FeRh and MnRh compounds feature a first-order metamagnetic phase transition between antiferromagnetic and ferromagnetic order in the vicinity of room temperature, exhibiting interconnected structural, magnetic, and electronic order parameters. We show that these two alloys can be combined to form hybrid metamagnets in the form of sputter-deposited superlattices and alloys on single-crystalline MgO substrates. Despite being structurally different, the magnetic behavior of the alloys with substantial Mn content resembles that of the FeRh/MnRh superlattices in the ultrathin individual layer limit. For FeRh/MnRh superlattices, dissimilar lattice distortions of the constituent FeRh and MnRh layers at the antiferromagnetic–ferromagnetic transition cause double-step transitions during cooling, while the magnetization during the heating branch shows a smooth, continuous trend. For $Fe_{50-x}Mn_xRh_{50}$ alloy films, the substitution of Mn at the Fe sites introduces an effective tensile in-plane strain and magnetic frustration in the highly ordered epitaxial films, largely influencing the phase transition temperature T_M (by more than 150 K). In addition, Mn acts as a surfactant, enabling the growth of continuous thin films at higher temperatures. Thus, the introduction of hybrid FeRh–MnRh systems with adjustable parameters provides a pathway for the realization of tunable spintronic devices based on magnetic phase transitions.

OPERA Work Group

WG1

Statistics of nucleation and growth of single monolayers in nanowires: Towards a deterministic regime



Abstract

The vapor–liquid–solid growth of semiconductor nanowires proceeds via the sequential nucleation and extension of biatomic monolayers at the interface between the solid wire and a liquid catalyst nanodroplet. In the case of III–V compounds, this mother phase contains only a small concentration of the volatile group V atoms. The growth regime where there is not enough such atoms available in the liquid at nucleation to complete a whole monolayer is studied experimentally and theoretically. Each monolayer cycle then consists in the rapid formation of a partial monolayer, followed by a slower propagation stage and by a waiting time preceding the next nucleation. The propagation and waiting times of long sequences of monolayers are measured in situ in a transmission electron microscope at three growth temperatures, in a single GaAs nanowire. The process is modeled and the statistics of the characteristic times are computed numerically and analytically. At low temperature, the weakness of group V desorption from the liquid should lead to a constant total monolayer cycle time, despite the stochasticity of the nucleation events. The modeling of the experiments yields values of several crucial growth parameters and provides guidance for the growth of nanowires in a deterministic regime.

Reference: physica status solidi (RRL) - Rapid Research Letters 16, 2100647 (2022). DOI 10.1002/pssr.202100647

Authors: F. Glas, F. Panciera, J.-C. Harmand

*Laboratories: C2N **(Fr)***

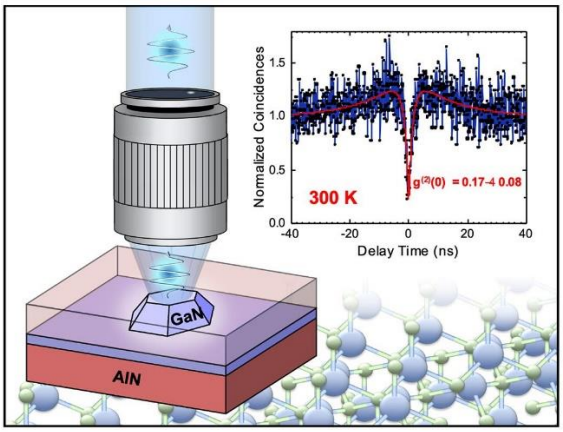
Techniques: MBE, in situ TEM, growth modelling

Materials: GaAs nanowires

OPERA Work Group

WG1

Single photon emission and recombination dynamics in self-assembled GaN/AlN quantum dots



Abstract

GaN/AlN quantum dots (QDs) are a promising system for achieving single photon emission at room temperature. Stranski-Krastanov GaN 3D-islands were synthesized on AlN template using molecular beam epitaxy. We studied the photoluminescence (PL) properties of a single GaN/AlN QD for temperatures ranging from 5 to 300 K. We measured the single photon purity and determined g(2)(0) values of 0.05 ± 0.02 at 5 K and 0.17 ± 0.08 at 300 K, respectively. We then performed temperature dependent time-resolved photoluminescence measurements (TRPL) on a QD ensemble and investigated the exciton recombination dynamics. TRPL transients display a bi-exponential feature with short- and long-lived components that persist in the low excitation regime. From the temperature insensitivity of the long-lived excitonic component, we first discard the interplay of dark-to-bright state refilling in the exciton recombination process. Besides, this temperature independent behavior also highlights the lack of nonradiative exciton recombination, a direct consequence of the strong carrier confinement. Overall, our results support GaN QDs as a potential single-photon source system for quantum applications at room temperature.

Reference: Light: Science & Applications 11:114 (2022); DOI: 10.1038/s41377-022-00799-4

Authors: J. Stachurski, S. Tamariz, G. Callsen, R. Butté, and N. Grandjean

Laboratories: LASPE-EPFL (CH)

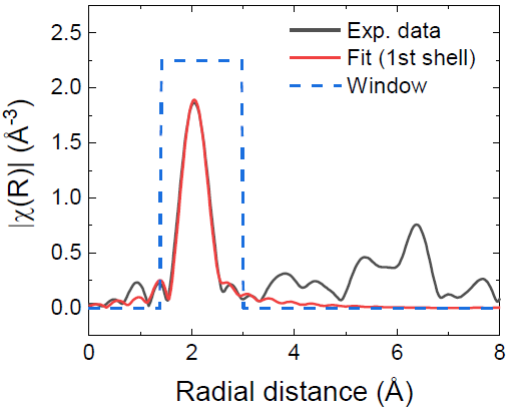
Techniques: MBE, PL, TRPL

Materials: GaN semiconductors

OPERA Work Group

WG1

Low temperature epitaxy of in situ Ga doped $Si_{1-x}Ge_x$: dopant incorporation, structural and electrical properties



Reference: *ECS Transactions, 109 (4) 135-140 (2022)*
DOI 10.1149/10904.0249ecst

Authors: *G. Rengo, C. Porret, A. Hikavyy, G. Coenen, M. Ayyad, R. J. H. Morris, S. Pollastri, D. Oliveira De Souza, D. Grandjean, R. Loo, and A. Vantomme*

Laboratories: *KU Leuven **(Be)**, Imec **(Be)**, FWO **(Be)**, Elettra-Sincrotrone Trieste **(It)***

Techniques: *RPCVD, SEM, HRXRD, XRR, SIMS, m4pp, micro-Hall, EXAFS,*

Materials: *SiGe:Ga, Ge:Ga semiconductors*

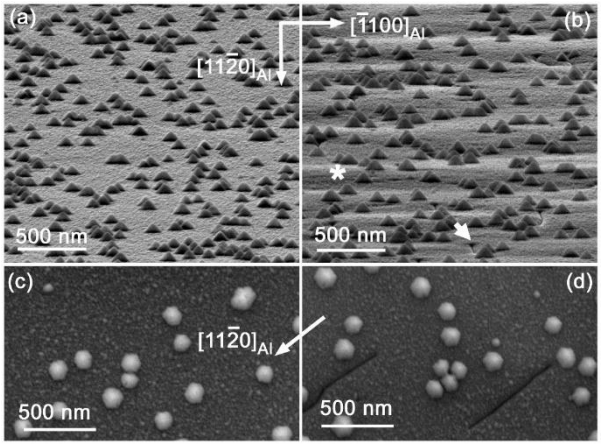
Abstract

The effect of the growth temperature and the Ga precursor flow on the epitaxy of Si1-xGex:Ga is studied. These parameters are found to have a significant impact on the Ga surface segregation behavior. In particular, Ga in situ doping impacts the growth rate of the epilayer, the Si1-xGex alloy composition, and the onset of strain relaxation. The growth temperature can be used to modulate the Ga segregation, enabling the deposition of materials with enhanced dopant concentrations and improved electrical properties. The Ga local atomic environment was studied in both a Si0.4Ge0.6:Ga and a Ge:Ga sample by X-ray absorption fine structure. The local environment of the Ga determined confirmed that the majority of dopants occupy a substitutional position within the lattice.

OPERA Work Group
WG1

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

In(Ga)N 3D growth on GaN-buffered on-axis and off-axis (0001) sapphire substrates by MOCVD



Reference: *Nanomaterials* *12*(19), 3496 (2022); *DOI:* https://doi.org/10.3390/nano12193496

Authors: *Rosová, A., Dobročka, E., Eliáš, P., Hasenöhrl, S., Kučera, M., Gucmann, F., and* Kuzmík J.

Laboratories: *Inst. El. Eng., Slovak Academy of Sci.* ***(Sk)***

Techniques: *MOVPE, SEM, TEM, XRD, PL,*

Materials: *GaN, InN.*

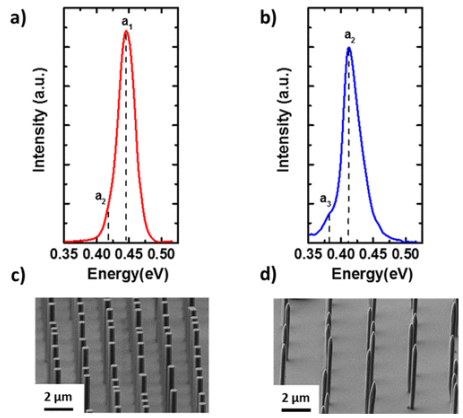
Abstract

In(Ga)N epitaxial layers were grown on on-axis and off-axis (0001) sapphire substrates with an about 1100 nm-thick GaN buffer layer stack using organometallic chemical vapour deposition at 600 °C. The In(Ga)N layers consisted of a thin (~10-25 nm) continuous layer of small conical pyramids in which large conical pyramids with the approximate height of 50-80 nm were randomly distributed. The large pyramids were grown above the edge-type dislocations which originated in the GaN buffer; the dislocations did not penetrate the large, isolated pyramids. The large pyramids were well crystallized and relaxed with a small quantity of defects, such as dislocations, preferentially located at the contact zones of adjacent pyramids. The low temperature (6.5 K) photoluminescence spectra showed one clear maximum at 853 meV with a full width at half maximum (FWHM) of 75 meV and 859 meV with a FWHM of 80 meV for the off-axis and on-axis samples, respectively.

OPERA Work Group

WG1 & WG2

Selective Area Growth by Hydride Vapor Phase Epitaxy and Optical Properties of InAs Nanowire Arrays



Reference: *Cryst. Growth Des. 2021, 21, 5158−5163;* *DOI:* 10.1021/acs.cgd.1c00518

Authors: *G. Grégoire, M. Zeghouane, C. Goosney, N. I. Goktas, P. Staudinger, H. Schmid, K. E. Moselund, T. Taliercio, E. Tournié, A. Trassoudaine, E. Gil, R. R. LaPierre, and Y. André*

Laboratories: *Institut PASCAL* ***(Fr)****, McMaster University* ***(Ca)****, IBM* ***(Ch)****, IES* ***(Fr)***

Techniques: *HVPE, SEM, PL, FTIR*

Materials: *InAs/Si(111)), InAs/GaAs(111)B*

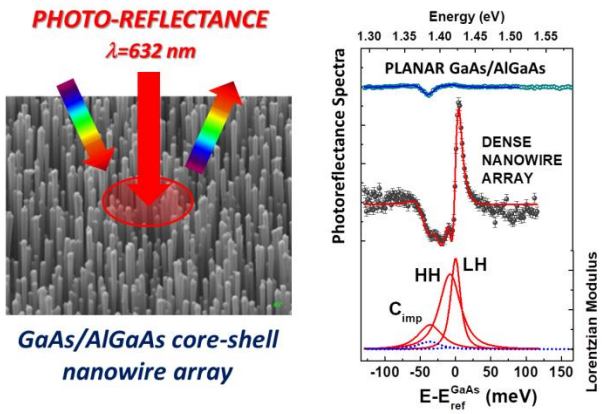
Abstract

We report on the selective area growth of InAs nanowires (NWs) by the catalyst-free vapor−solid method. Well-ordered InAs NWs were grown on GaAs(111)B and Si(111) substrates patterned with a dielectric mask using hydride vapor phase epitaxy (HVPE). Vertical and high aspect ratio InAs NWs with a hexagonal shape were grown on both GaAs and Si substrates. The impact of the growth conditions on the InAs morphology was investigated. The final shape of the InAs crystal was tuned from a NW to a nanoplatelet by controlling growth conditions such as growth temperature, vapor phase composition, and mask pattern. The influence of the aperture size on the nucleation density and then on the morphology of InAs is discussed. Small openings resulted in the formation of a single nucleus per hole, which was then converted to a NW. For larger apertures, the number of nuclei increased, leading to both three-dimensional crystals and NWs. The effect of growth temperature and the III/V ratio on the kinetics and thermodynamics of InAs growth is also discussed. The growth was first optimized on a GaAs(111)B substrate and then performed on Si, which is more suitable to develop devices. Finally, the absorbance and photoluminescence measurements were carried out on the InAs NW arrays, demonstrating the high potential of HVPE-grown InAs NWs for future multispectral photo-detection devices.

OPERA Work Group

WG1 & WG2

Enhanced Optical Absorption of GaAs Near-Band-Edge Transitions in GaAs/AlGaAs Core-Shell Nanowires: Implications for Nanowire Solar Cells



Reference: *ACS Appl. Nano Mater. 5, 18149−18158 (2022); DOI: 10.1021/acsanm.2c04044*

Authors: *A. Cretì, P. Prete, N. Lovergine, and M. Lomascolo*

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

Techniques: *MOVPE, Photo-Reflectance, FESEM, Growth Modelling.*

Materials: *(Al)GaAs semiconductor core-shell nanowires*

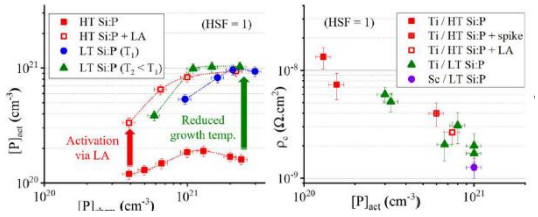
Abstract

Dense arrays of core−shell nanowires possess great potential as super-absorptive media for fabrication of efficient solar cells. We report on GaAs near-band-edge absorption properties of free-standing GaAs−AlGaAs core−shell nanowires having different shell thicknesses, by detailed line-shape analyses of room-temperature photoreflectance (PR) spectra, employing first-derivative Gaussian and Lorentzian models of the GaAs complex dielectric function. Line-shape analyses of the nanowire PR spectra returned a doublet of resonance lines at energies between 1.410 and 1.422 eV, ascribed to strain-split heavy- and light-hole exciton absorption transitions in the GaAs nanowire cores. The optical oscillator strengths of exciton resonances evaluated by Lorentzian analyses of PR features showed a significant enhancement (up to 30×) of GaAs band-edge optical absorption in nanowires with respect to the reference planar structure. Additionally, values of integrated Lorentzian moduli were normalized to the total GaAs core volume fill fraction (estimated in the range 0.5−7.0% with respect to a planar layer of the same height) within each nanowire ensemble, achieving a first ever experimental estimate of the GaAs near band-edge absorption enhancement factor for GaAs−AlGaAs core−shell nanowires in the range 22−190, depending on the nanowire inner core−shell structure. Such strong absorption enhancement is ascribed to improved wave-guiding of incident light into the GaAs cores by the surrounding AlGaAs shell (its average thickness being estimated between ~14 and 100 nm in the present nanostructures).

OPERA Work Group

WG1 and WG2

Low temperature source / drain epitaxy and functional silicides: essentials for ultimate contact scaling



Reference: *2022 International Electron Devices Meeting (IEDM)*, San Francisco, CA, USA, 2022, pp. 34.1.1-34.1.4, doi: 10.1109/IEDM45625.2022.10019501.

Authors: *C. Porret, J.-L. Everaert, M. Schaekers, L.-A. Ragnarsson, A. Hikavyy, E. Rosseel, G. Rengo, R. Loo, R. Khazaka, M. Givens, X. Piao, S. Mertens, N. Heylen, H. Mertens, C. Toledo de Carvalho Cavalcante, G. Sterckx, S. Brus, A. Nalin Mehta, M. Korytov, D. Batuk, P. Favia, R. Langer, G. Pourtois, J. Swerts, E. Dentoni Litta, and N. Horiguchi*

Laboratories: *Imec (Be), ASM (Be)*

Techniques: *RPCVD, MR-CTLM, TLM, SEM, Hall, TEM, SIMS*

Materials: *Si:P, SiGe:B semiconductors, Ti, Gd, Sc, Hf, Mo, Nb silicides*

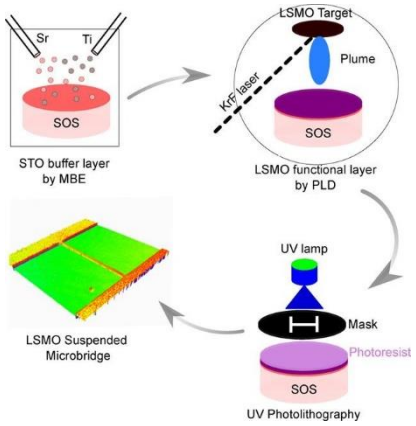
Abstract

Low temperature $Si_{1-x}Ge_x$ source-drain epitaxy processes are associated with exploratory contact metals to identify stacks alleviating access resistance issues in modern logic devices. TiN/W metal-to-metal interfaces featuring contact resistivities $<5 \times 10^{-10}$ Ω.cm² demonstrate the resolution of the test vehicle and extraction methods. Amongst the different systems investigated, Sc/Si:P yields ~1.3×10⁻⁹Ω·cm2, which represents a ~35% reduction with respect to the Ti/Si:P reference. This confirms that doping levels in Si:P are sufficient to achieve significant performance gains. Analyses of Sc/Si:P stacks reveal the material properties and reaction mechanisms responsible for the contact resistivity reduction.

OPERA Work Group

WG1 , WG2

Integration of epitaxial $La_{2/3}Sr_{1/3}MnO_3$ thin films on Silicon-on-Sapphire substrate



Reference: *Applied Surface Science, Vol. 579, 152095 (2022); doi: 10.1016/j.apsusc.2021.152095*

Authors: *S.K. Chaluvadi, Z. Wang, L.M. Carvalho de Araujo, P. Orgiani, V. Polewczyk, G. Vinai, O. Rousseau, V. Pierron, A. Pautrat, B. Domenges, D.G. Schlom, L. Méchin*

Laboratories: *GREYC, Caen **(Fr)**, IOM-CNR, Trieste **(It)**, Cornell University, Ithaca **(US)**, CNR-SPIN, UOS Salerno **(It)**, CRISMAT, Caen **(Fr)***

Techniques: *MBE, PLD*

Materials: *$La_{2/3}Sr_{1/3}MnO_3$, $SrTiO_3$, Silicon, Sapphire*

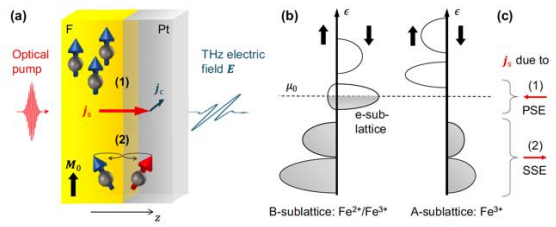
Abstract

We report the integration of high-quality epitaxial $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) thin films onto $SrTiO_3$ buffered Silicon-on-Sapphire (SOS) substrates by combining state-of-the-art thin film growth techniques such as molecular beam epitaxy and pulsed laser deposition. Detailed structural, magnetic and electrical characterizations of the LSMO/STO/SOS heterostructures show that the LSMO film properties are competitive with those directly grown on oxide substrates. X-ray magnetic circular dichroism measurements on Mn L2,3 edges show strong dichroic signal at room temperature, and angular-dependent in-plane magnetic properties by magneto-optical Kerr magnetometry reveal isotropic magnetic anisotropy. Suspended micro-bridges were thus finally fabricated by silicon micromachining, thus demonstrating the potential use of integrating LSMO magnetic layer on industrially compatible SOS substrates for the development of applicative MEMS devices.

OPERA Work Group

WG1 , WG2

Transition of laser-induced terahertz spin currents from torque- to conduction-electron-mediated transport



Reference: *PHYSICAL REVIEW B 105, 184408 (2022); DOI; 10.1103/PhysRevB.105.1844*

Authors: *P. Jiménez-Cavero, O. Gueckstock, L. Nádvorník, I. Lucas, T. S. Seifert, M. Wolf, R. Rouzegar, P. W. Brouwer, S. Becker , G. Jakob , M. Kläui, C. Guo, C. Wan, X. Han, Z. Jin, H. Zhao, D. Wu, L. Morellón and T. Kampfrath.*

Laboratories: *Freie Universität Berlin **(De)**, Instituto de Nanociencia y Materiales de Aragón **(Es)**, Universidad de Zaragoza-CSIC **(Es)**, Charles University, Institut für Physik, Johannes Gutenberg-Universität Mainz **(De)**, Beijing National Laboratory for Condensed Matter Physics **(Cn)**, University of Chinese Academy of Sciences,**(Cn)** Shanghai Key Lab of Modern Optical Systems, **(Cn)** University of Shanghai for Science and Technology and National Laboratory of Solid State Microstructures, Nanjing University, **(Cn).***

Techniques: *PLD, Sputtering and LPE..*

Materials: *YIG, GIG, Fe3O4, γ-Fe3O4, Fe and Pt.*

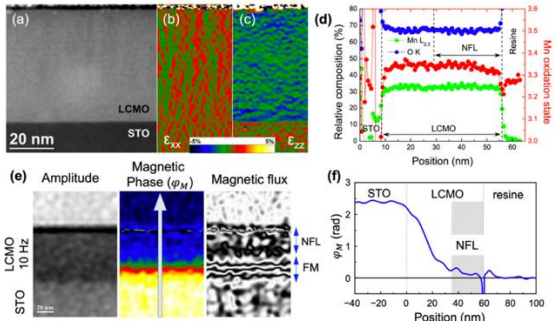
Abstract

Spin transport is crucial for future spintronic devices operating at bandwidths up to the terahertz range. In F|N thin-film stacks made of a ferromagnetic/ferrimagnetic layer F and a normal-metal layer N, spin transport is mediated by (1) spin-polarized conduction electrons and/or (2) torque between electron spins. To identify a crossover from (1) to (2), we study laser-driven spin currents in F|Pt stacks where F consists of model materials with different degrees of electrical conductivity. For the magnetic insulators yttrium iron garnet, gadolinium iron garnet (GIG) and γ -Fe2O3, identical dynamics is observed. It arises from the terahertz interfacial spinSeebeck effect (SSE), is fully determined by the relaxation of the electrons in the metal layer, and provides a rough estimate of the spin-mixing conductance of the GIG/Pt and γ -Fe2O3/Pt interfaces. Remarkably, in the half-metallic ferrimagnet Fe3O4 (magnetite), our measurements reveal two spin-current components with opposite direction. The slower, positive component exhibits SSE dynamics and is assigned to torque-type magnon excitation of the A- and B-spin sublattices of Fe3O4. The faster, negative component arises from the pyrospintronic effect and can consistently be assigned to ultrafast demagnetization of minority-spin hopping electrons. This observation supports the magneto-electronic model of Fe3O4. In general, our results provide a route to the contact-free separation of torque- and conduction-electron-mediated spin currents…

OPERA Work Group

WG1 & WG2

Spin Glass State in Strained La2/3Ca1/3MnO3 Thin Films



Abstract

Epitaxial strain modifies the physical properties of thin films deposited on single-crystal substrates. In a previous work, we demonstrated that in the case of La2/3Ca1/3MnO3 thin films the strain induced by the substrate can produce the segregation of a non-ferromagnetic layer (NFL) at the top surface of ferromagnetic epitaxial La2/3Ca1/3MnO3 for a critical value of the tetragonality τ defined as $\tau = |c\text{-}a|a$, of $\tau_C \approx 0{,}024$. Although preliminary analysis suggested its antiferromagnetic nature, to date a complete characterization of the magnetic state of such an NFL has not been performed. Here, we present a comprehensive magnetic characterization of the strain-induced segregated NFL. The field-cooled magnetic hysteresis loops exhibit an exchange bias mechanism below $T \approx 80$ K, which is well below the Curie temperature of the ferromagnetic La2/3Ca1/3MnO3 layer. The exchange bias and coercive fields decay exponentially with temperature, which is commonly accepted to describe spin-glass (SG) behavior. The signatures of slow dynamics were confirmed by slow spin relaxation over a wide temperature regime. Low-energy muon spectroscopy experiments directly evidence the slowing down of the magnetic moments below T~100 K in the NFL. The experimental results indicate the SG nature of the NFL. This SG state can be understood within the context of the competing ferromagnetic and antiferromagnetic interactions of similar energies.

Reference: *Nanomaterials 2022, 12, 3646. DOI: doi.org/10.3390/nano12203646*

Authors: *I. Lucas, N. Marcano, T.s Proksch, C. Magén, R. Corcuera, L. Morellón, J. M. De Teresa, M. Ricardo Ibarra and P. A. Algarabel*

Laboratories: *Instituto de Nanociencia y Materiales de Aragón (INMA) **(Es)**, CSIC-Universidad de Zaragoza, **(Es)** Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut **(Ch)**, Laboratorio de Microscopías Avanzadas (LMA), Universidad de Zaragoza. **(Es)***

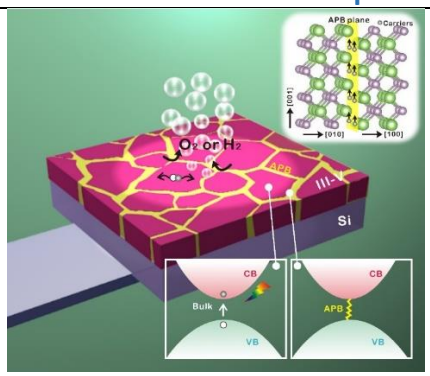
Techniques: *PLD*

Materials: *La2/3Ca1/3MnO3*

OPERA Work Group

WG1 & WG2

Epitaxial III–V/Si Vertical Heterostructures with Hybrid 2D-Semimetal/Semiconductor Ambipolar and Photoactive Properties



Abstract

Here, it is demonstrated that epitaxial bi-domain III–V/Si are hybrid structures, composed of bulk photo-active semiconductors with 2D topological semi-metallic vertical inclusions, endowed with ambipolar properties. By combining structural, transport, and photoelectrochemical characterizations with first-principle calculations, it is shown that the bi-domain III–V/Si materials are able within the same layer to absorb light efficiently, separate laterally the photo-generated carriers, transfer them to semimetal singularities, and ease extraction of both electrons and holes vertically, leading to efficient carrier collection. Besides, the original topological properties of the 2D semi-metallic inclusions are also discussed. This comb-like heterostructure not only merges the superior optical properties of semiconductors with good transport properties of metallic materials, but also combines the high efficiency and tunability afforded by III–V inorganic bulk materials with the flexible management of nano-scale charge carriers usually offered by blends of organic materials. Physical properties of these novel hybrid heterostructures can be of great interest for energy harvesting, photonic, electronic or computing devices.

Reference: *Advanced Science 2022, 9, 2101661; DOI: 10.1002/advs.202101661*

Authors: *L. Chen, Y. Léger, G. Loget, M. Piriyev, I. Jadli, S. Tricot, T. Rohel, R. Bernard, A. Beck, J. Le Pouliquen, P. Turban, P. Schieffer, C. Levallois, B. Fabre, L. Pedesseau, J. Even, N. Bertru, and C. Cornet*

Laboratories: *Institut FOTON **(Fr)**, ISCR **(Fr)**, IPR **(Fr)***

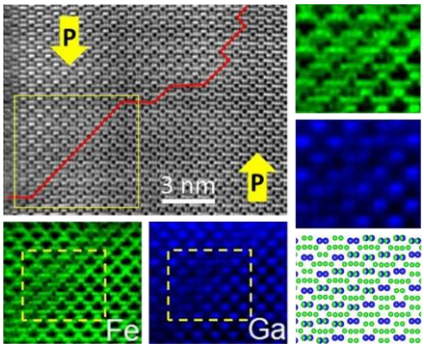
Techniques: *MBE, SEM, Hall, C-AFM, PEC, Mott-Schottky, DFT*

Materials: *GaP/Si(001), GaPSb/Si(001), GaPAs/Si(001), GaP, antiphase boundaries*

OPERA Work Group

WG1 & WG2

Unveiling unconventional ferroelectric switching in multiferroic $Ga_{0.6}Fe_{1.4}O_3$ thin films through multiscale electron microscopy investigations



Reference: *Acta Materialia 2022, 240, 118337; DOI: 10.1016/j.actamat.2022.118337*

Authors: *A. Demchenko, S. Homkar, C. Bouillet, C. Lefèvre, F. Roulland, D. Preziosi, G. Versini, C. Leuvrey, P. Boullay, X. Devaux, N. Viart.*

Laboratories:

*Université de Strasbourg, CNRS, IPCMS **(Fr),** Normandie Université, CNRS, CRISMAT, **(Fr),** Université de Lorraine, CNRS, IJL **(Fr)***

Techniques : *PLD, PEDT, HR-STEM-EELS*

Materials: *Multiferroic gallium ferrite $Ga_{0.6}Fe_{1.4}O_3$*

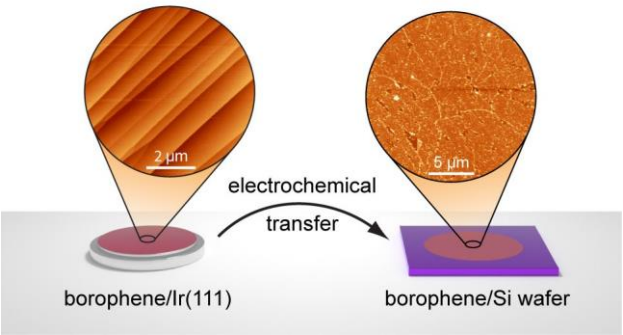
Abstract

Understanding the polarization switching mechanisms at play in ferroelectric materials is crucial for their exploitation in electronic devices. The conventional centrosymmetric reference structure-based mechanism which accounts for ferroelectricity in most of the usual displacive ferroelectric materi- als is too energy-demanding for some newly diagnosed ferroelectric materials such as the $Ga_{2-x}Fe_xO_3$ ($0.8 \leq x \leq 1.4$) compounds. Some alternative theoretical propositions have been made and need experimental confirmation. A dual-scale electron microscopy study is performed on pulsed laser deposited epitaxial thin films of the $Ga_{0.6}Fe_{1.4}O_3$ multiferroic compound. A wide scale precession-assisted electron diffraction tomography study first allows the determination of the structure the compound adopts in thin films, and even permits the refinement of the atomic positions within this structure. Cationic mobility is suggested for two of the atomic positions through the existence of extra electronic density. A local in situ high resolution scanning transmission electron microscopy study then allows confirming these mobilities by directly spotting the cationic displacements on successively acquired images. The whole study confirms an unconventional switching mechanism via local domain wall motion in this compound.

OPERA Work Group

WG1 & WG2

Macroscopic single-phase monolayer borophene on arbitrary substrates



Reference: *ACS Appl. Mater. Interfaces 14, 21727 (2022); DOI: 10.1021/acsami.2c03678*

Authors: *B. Radatović, V. Jadriško, S. Kamal, M. Kralj, D. Novko, N. Vujičić, M. Petrović*

Laboratories: *Surfaces, interfaces and 2D materials research group, Institute of Physics Zagreb **(Cro)***

Techniques: *LEED, AFM, SEM, Raman, DFT, CVD, electrochemical transfer*

Materials: *borophene, Si wafer*

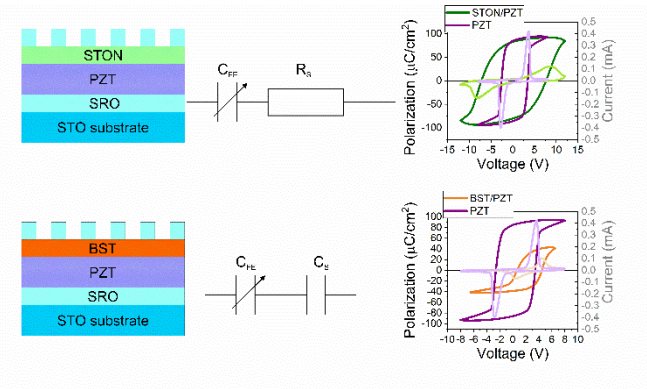
Abstract

A major challenge in the investigation of all 2D materials is the development of synthesis protocols and tools which would enable their large-scale production and effective manipulation. The same holds for borophene, where experiments are still largely limited to in situ characterizations of small-area samples. In contrast, our work is based on millimeter-sized borophene sheets, synthesized on an Ir(111) surface in ultrahigh vacuum. Besides high-quality macroscopic synthesis, as confirmed by low-energy electron diffraction (LEED) and atomic force microscopy (AFM), we also demonstrate a successful transfer of borophene from Ir to a Si wafer via electrochemical delamination process. Comparative Raman spectroscopy, in combination with the density functional theory (DFT) calculations, proved that borophene's crystal structure has been preserved in the transfer. Our results demonstrate successful growth and manipulation of large-scale, single-layer borophene sheets with minor defects and ambient stability, thus expediting borophene implementation into more complex systems and devices.

OPERA Work Group

WG1 & WG2

Negative Capacitance and Switching Dynamics Control Via Non-Ferroelectric Elements



Abstract

Complex ferroelectric structures with dielectric inter-layers may become possible alternatives for neuromorphic computing and low-power field-effect transistors since they exhibit multiple polarization states and negative capacitance. However, the effects on the switching characteristics due to the electric properties of the non-ferroelectric circuit element have not been clearly evaluated so far. A high-resistance or low-capacitance element is usually associated with an increased depolarization field and eventually with suppression of polarization but without further consideration of the electrostatic differences. Therefore, we show that switching behavior is dramatically changed if the non-FE element is a resistive component or a capacitive one. This is reflected by either an increased apparent coercive field or imprint, respectively. A negative capacitance regime was observed at different moments but strongly depends on the nature of the non-ferroelectric element. The voltage on the ferroelectric component remains constant during switching, which is a fingerprint of the system passing through non-equilibrium states. Therefore, we propose an algorithm to recover the S-shape of polarization dependence on the ferroelectric internal voltage during the slowed transition between the two stable states of polarization.

Reference: *ACS Appl. Energy Mater. 2022, 5, 3, 3307–3318* https://doi.org/10.1021/acsaem.1c03890

Authors: *A.G. Boni, R. Patru, L.D. Filip, C. Chiril, I. Pasuk, I. Pintilie, L. Pintilie*

Laboratories: *National Institute of Materials Physics,* ***(Ro)***

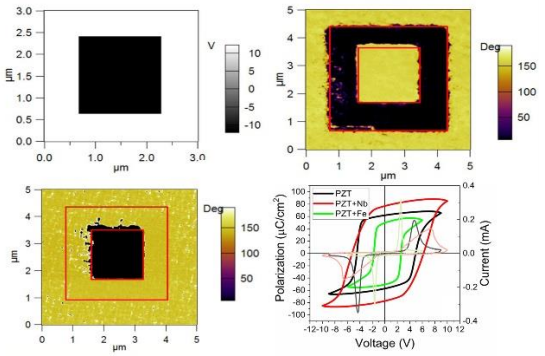
Techniques: *PLD, HR-TEM, HR-XRD.*

Materials: *PZT, SRO, Nb doped STO, BST.*

OPERA Work Group

WG1 & WG2

Controlling polarization direction in epitaxial $Pb(Zr_{0.2}Ti_{0.8})O_3$ films through Nb (n-type) and Fe (p-type) doping



Abstract

In this study, the authors investigated the impact of 1% Fe and Nb doping on the electrical characteristics of epitaxial PZT films. They used PLD to deposit the epitaxial films from Fe and Nb doped targets and found that the electrical properties of Fe and Nb doped PZT were significantly different from each other. Specifically, they found that the polarization orientation in the as-grown layers differed between the two types of doping. PFM was used to reveal that the polarization of the as-grown Nb-doped PZT was oriented upward, while that of the Fe-doped PZT was mostly oriented downward. The authors explained this difference as a result of the modification of the carriers involved in the growth-induced compensation of the depolarization field in terms of their conduction type and, consequently, their sign.

The authors suggest that their findings may have implications for the development of p-n ferroelectric homojunctions and that PFM can be used to identify the type of conduction in PZT based on the dominant direction of polarization in the as-grown films. Overall, this study provides important insights into the role of doping on the electrical properties of PZT films and the potential for manipulating polarization orientation through changes in doping type.

Reference: *Sci Rep* **12**, 755 (2022); https://doi.org/10.1038/s41598-022-04802-1

Authors: *C. F. Chirila, V. Stancu, G. A. Boni, I. Pasuk, L. Trupina, L. D. Filip, C. Radu, I. Pintilie, L. Pintilie*

Laboratories: *National Institute of Materials Physics,* ***(Ro)***

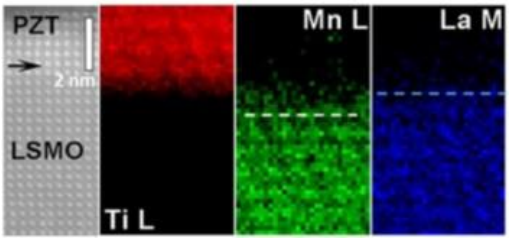
Techniques: *PLD, HR-TEM, HR-XRD, PFM*

Materials: *doped ferroelectric, PZT*

OPERA Work Group

WG1 & WG2

Ferroelectricity modulates polaronic coupling at multiferroic interfaces



Reference: *Commun Phys* **5**, 209 (2022) ; DOI : https://doi.org/10.1038/s42005-022-00983-3

Authors: *M. A. Husanu, D. G. Popescu, F. Bisti, L. M. Hrib, L. D. Filip, I. Pasuk, R. Negrea, M. C. Istrate, L. Lev, T. Schmitt, L. Pintilie, A. Mishchenko, C. M. Teodorescu & V. N. Strocov*

Laboratories: *National Institute of Materials Physics,* ***(Ro)***

Techniques: *PLD, X-ray photoemission*

Materials: *LSMO, PZT, BTO*

Abstract

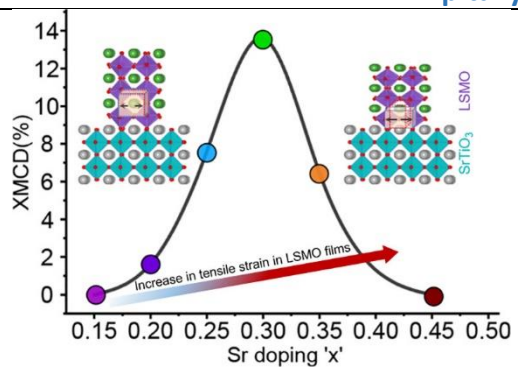
The k-resolved soft X-ray photoemission experiments on epitaxial multiferroic LSMO/$BaTiO_3$ and LSMO/$PbZrTiO_3$ heterostructures have provided important insights into the electronic properties of the interface between the ferroelectric layer and the LSMO layer. By carefully preparing these epitaxial heterostructures, the researchers were able to probe the electronic structure of the buried interface using soft X-ray photoemission.The experiments revealed that the interface between the ferroelectric layer and the LSMO layer induces a band-dependent electron/hole accumulation/depletion, which is modulated by the strength of the electron-phonon interaction (EPI) and leads to changes in conductivity. This suggests that the interface can be used to tune the functionality of the heterostructure.

It is important to note that the ferroelectric layer in these heterostructures is thin enough to access the electronic structure of the interface using soft X-ray photoemission, but also thick enough to maintain its ferroelectric character. This is because materials like PZT and BTO lose their ferroelectricity below a critical thickness of ~3-6 unit cells. These findings have opened up new avenues for the development of oxide electronic, spintronic, and superconducting devices that rely on the multifaceted effect of ferroelectric polarization on the electronic properties of the interface.

OPERA Work Group

WG1 & WG2

Electronic Properties of Fully Strained $La_{1-x}Sr_xMnO_3$ Thin Films Grown by Molecular Beam Epitaxy ($0.15 \leq x \leq 0.45$)



Reference: *ACS Omega 7, 17, 14571–14578 (2022);* *DOI:* 10.1021/acsomega.1c06529

Authors: *S.K. Chaluvadi, V. Polewczyk, A.Y. Petrov, G. Vinai, L. Braglia, J. M. Diez, V. Pierron, P. Perna, L. Méchin, P. Torelli, P. Orgiani*

Laboratories: *GREYC, Caen* ***(Fr)****; IOM−CNR, Trieste* ***(It)****; IMDEA-Nanociencia, Madrid* ***(Es).***

Techniques: *MBE*

Materials: *$La_{2/3}Sr_{1/3}MnO_3$, $SrTiO_3$*

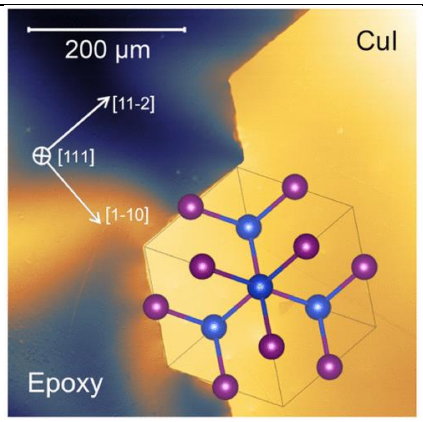
Abstract

The structural, electronic, and magnetic properties of Sr-hole-doped epitaxial $La_{1-x}Sr_xMnO_3$ ($0.15 \leq x \leq 0.45$) thin films deposited using the molecular beam epitaxy technique on 4° vicinal STO (001) substrates are probed by the combination of X-ray diffraction and various synchrotron-based spectroscopy techniques. The structural characterizations evidence a significant shift in the LSMO (002) peak to the higher diffraction angles owing to the increase in Sr doping concentrations in thin films. The nature of the LSMO Mn mixed-valence state was estimated from X-ray photoemission spectroscopy together with the relative changes in the Mn L2,3 edges observed in X-ray absorption spectroscopy (XAS), both strongly affected by doping. CTM4XAS simulations at the XAS Mn L2,3 edges reveal the combination of epitaxial strain, and different MnO6 crystal field splitting give rise to a peak at ~641 eV. The observed changes in the occupancy of the eg and the t2g orbitals as well as their binding energy positions toward the Fermi level with hole doping are discussed. The room-temperature magnetic properties were probed at the end by circular dichroism.

OPERA Work Group

WG1 & WG2

Suppression of Rotational Domains of CuI Employing Sodium Halide Buffer Layers



Reference: *ACS Appl. Mater. Interfaces 2022, 14, 12350; DOI: https://doi.org/10.1021/acsami.1c24432*

Authors: *P. Storm, K. Karimova, M. S. Bar, S. Selle, H. von Wenckstern, M. Grundmann, and M. Lorenz*

Laboratories: *Univ. Leipzig **(De)**, FhG IMWS Halle **(De)***

Techniques: *PLD, XRD, LSM, SEM, AFM, Hall*

Materials: *CuI, NaCl, NaBr*

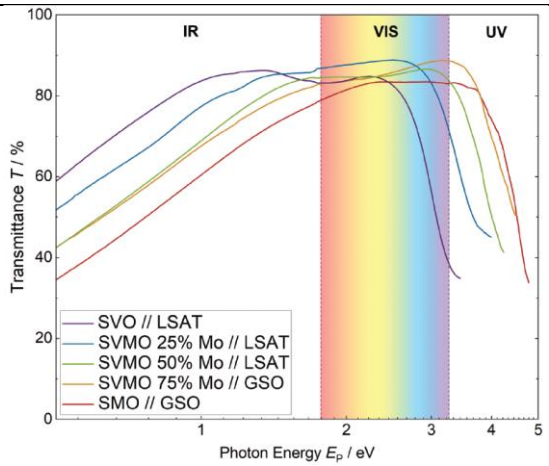
Abstract

The occurrence of rotational domains is a well-known issue for copper iodide (CuI) that naturally occurs for growth on popular substrates like sapphire. However, this has detrimental effects on the thin film quality like increasing surface roughness or deteriorated transport characteristics due to grain boundary scattering. Utilizing pulsed laser deposition and the in situ growth of sodium chloride (NaCl) and sodium bromide (NaBr) template layers, studies were performed on their potential on suppressing the formation of rotational domains of CuI on c-plane sapphire and SrF_2(111) substrates. Corresponding samples were investigated concerning their epitaxial properties and further characterized regarding (volume) crystalline, morphological, and electrical properties. Particularly for NaBr template layers, fully single crystalline growth of CuI thin films was obtained and resulted in significantly reduced surface roughness of the CuI layer.

OPERA Work Group

WG1, WG2

Tailoring Optical Properties in Transparent Highly Conducting Perovskites by Cationic Substitution



Reference: *Advanced Materials 2023, 35, 202206605; DOI: 10.1002/adma.202206605*

Authors: *M. Mohammadi, R. Xie, N. Hadaeghi, A. Radetinac, A. Arzumanov, P. Komissinskiy, H. Zhang, and L. Alff*

Laboratories: *Institute of Materials Science, TU Darmstadt **(De)***

Techniques: *PLD, XRD, UV-Vis, Transport, DFT*

Materials: *$SrV_{1-x}Mo_xO_3$ on $GdScO_3$ and $(LaAlO_3)_{0.3}(Sr_2TaAlO_6)_{0.7}$ (LSAT)*

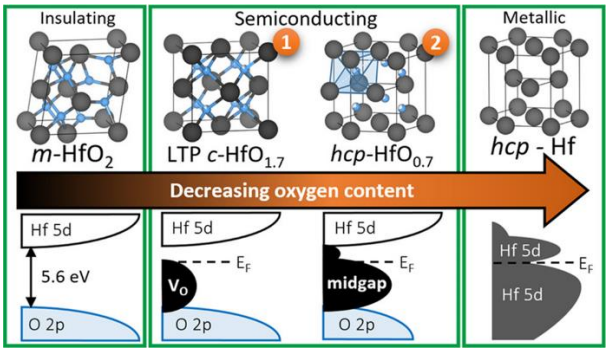
Abstract

$SrMoO_3$, $SrNbO_3$, and $SrVO_3$ are remarkable highly conducting d^1 (V, Nb) or d^2 (Mo) perovskite metals with an intrinsically high transparency in the visible. A key scientific question is how the optical properties of these materials can be manipulated to make them suitable for applications as transparent electrodes and in plasmonics. Here, it is shown how 3d/4d cationic substitution in perovskites tailors the relevant materials parameters, i.e., optical transition energy and plasma frequency. With the example of the solid-state solution $SrV_{1-x}Mo_xO_3$, it is shown that the absorption and reflection edges can be shifted to the edges of the visible light spectrum, resulting in a material that has the potential to outperform indium tin oxide (ITO) due to its extremely low sheet resistance. An optimum for x = 0.5, where a resistivity of 32 µΩcm (≈12 Ω sq−1) is paired with a transmittance above 84% in the whole visible spectrum is found. Quantitative comparison between experiments and electronic structure calculations show that the shift of the plasma frequency is governed by the interplay of d-band filling and electronic correlations. This study advances the knowledge about the peculiar class of highly conducting perovskites toward sustainable transparent conductors and emergent plasmonics.

OPERA Work Group

WG1 & WG2

Defect-Stabilized Substoichiometric Polymorphs of Hafnium Oxide with Semiconducting Properties



Reference: *ACS Applied Materials & Interfaces 2022, 14, 1, 1290;*
DOI: 10.1021/acsami.1c09451

Authors: *N. Kaiser, T. Vogel, A. Zintler, S. Petzold, A. Arzumanov, E. Piros, R. Eilhardt, L. Molina-Luna, and L. Alff*

Laboratories: *Institute of Materials Science, TU Darmstadt* ***(De)***

Techniques: *MBE, XRD, XPS, HR-TEM, Transport*

Materials: *HfO_2, $HfO_{1.5}$, $HfO_{0.7}$ on c-Al_2O_3*

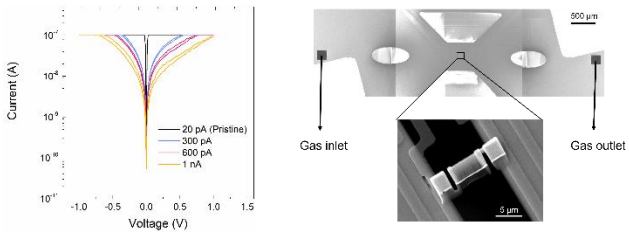
Abstract

Hafnium oxide plays an important role as a dielectric material in various thin-film electronic devices such as transistors and resistive or ferroelectric memory. The crystallographic and electronic structure of the hafnia layer often depends critically on its composition and defect structure. Here, we report two novel defect-stabilized polymorphs of substoichiometric HfO_{2-x} with semiconducting properties that are of particular interest for resistive switching digital or analog memory devices. The thin-film samples are synthesized by molecular beam epitaxy with oxygen engineering that allows us to cover the whole range of metallic Hf with oxygen interstitials to HfO_2. The crystal and defect structures, in particular of a cubic low-temperature phase c-$HfO_{1.7}$ and a hexagonal phase hcp-$HfO_{0.7}$ are identified by X-ray diffraction, in vacuo electron spectroscopic, and transmission electron microscopic methods. With the help of UV/Vis transmission data, we propose a consistent band structure model for the whole oxidation range involving oxygen vacancy-induced in-gap defect states. Our comprehensive study of engineered hafnia thin films has an impact on the design of resistive memory devices and can be transferred to chemically similar suboxide systems.

OPERA Work Group

WG1 & WG2

Effect of Induced Stimuli on the Leakage Current of Operative Oxide-based Devices inside a TEM



Reference: *Microscopy and Microanalysis 2022, 28, S1, 1, 820 - DOI: 10.1017/S1431927622003671*

Authors: *O. Recalde, T. Jiang, R. Eilhardt, A. Zintler, Y. Ruan, A. Arzumanov, T. van Omme, G. Pivak, H. H Perez-Garza, P. Komissinskiy, L. Alff, L. Molina-Luna*

Laboratories: *Institute of Materials Science, TU Darmstadt* ***(De)***, *DENSsolutions* ***(NL)***

Techniques: *PLD, MBE, HR-TEM*

Materials: *$SrTiO_3$, $BaSrTiO_3$, $SrMoO_3$*

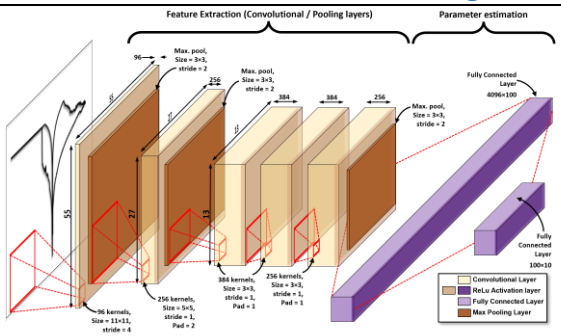
Abstract

Nanoelectronics devices are guided by their electrical performance under operative conditions. Therefore, a detailed understanding of the correlation between the electrical properties and the material structure at the nano and sub-nano levels is needed. In this way, microelectromechanical systems (MEMS) for in situ transmission electron microscopes (TEM) offer the possibility to perform multi-stimuli experiments comparable to real working conditions. However, to this date, biasing of e.g., Metal-Insulator-Metal (MIM) devices inside a TEM using MEMS-based chips has not been fully achieved due to its complex sample preparation and the generation of parasitic stray leakage paths. Here, a focused ion beam (FIB)-based preparation of TEM lamellas free of short-circuits is shown. Additionally, a study of the effect of induced stimuli on the device's leakage current during working conditions is also demonstrated.

OPERA Work Group

WG1 & WG2

Fast Fitting of the Dynamic Memdiode Model to the Conduction Characteristics of RRAM Devices Using Convolutional Neural Networks



Reference: *Micromachines. 2022; 13(11):2002.*
DOI : https://doi.org/10.3390/mi13112002

Authors: *F. L. Aguirre, E. Piros, N. Kaiser, T. Vogel, S. Petzold, J. Gehrunger, T. Oster, C. Hochberger, J.i Suñé, L. Alff, and E. Miranda*

Laboratories: *Institute of Materials Science, TU Darmstadt **(De)**, Universitat Autònoma de Barcelona **(Es)**, Department of Electrical and Information Engineering, TU Darmstadt **(De)***

Techniques: *MBE, SCS, simulation tools: ANN, CNN*

Materials: *Si/Al/TiN/Y_2O_{3-x}/Pt stacks*

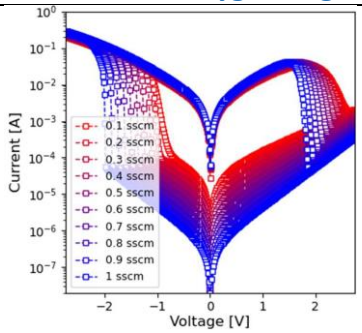
Abstract

In this paper, the use of Artificial Neural Networks (ANNs) in the form of Convolutional Neural Networks (AlexNET) for the fast and energy-efficient fitting of the Dynamic Memdiode Model (DMM) to the conduction characteristics of bipolar-type resistive switching (RS) devices is investigated. Despite an initial computationally intensive training phase the ANNs allow obtaining a mapping between the experimental Current-Voltage (I-V) curve and the corresponding DMM parameters without incurring a costly iterative process as typically considered in error minimization-based optimization algorithms. In order to demonstrate the fitting capabilities of the proposed approach, a complete set of I-Vs obtained from Y2O3-based RRAM devices, fabricated with different oxidation conditions and measured with different current compliances, is considered. In this way, in addition to the intrinsic RS variability, extrinsic variation is achieved by means of external factors (oxygen content and damage control during the set process). We show that the reported method provides a significant reduction of the fitting time (one order of magnitude), especially in the case of large data sets. This issue is crucial when the extraction of the model parameters and their statistical characterization are required.

OPERA Work Group

WG1 & WG2

Compact Model for Oxygen Engineered Yttrium Oxide-Based Resistive Switching Devices



Reference: *2022 IEEE 22nd International Conference on Nanotechnology (NANO), Palma de Mallorca, Spain, 2022, pp. 275-278, DOI: 10.1109/NANO54668.2022.9928654*

Authors: *F. Aguirre, E. Piros, L. Alff, C. Hochberger, J. Gehrunger, S. Petzold, N. Kaiser, E. Jalaguier, E. Nolot, C. Charpin-Nicolle, T. Vogel, L. Molina-Luna, J. Suñé, and E. Miranda.*

Laboratories: *Institute of Materials Science, TU Darmstadt **(De)**, Universitat Autònoma de Barcelona **(Es)**, Department of Electrical and Information Engineering, TU Darmstadt **(De)***

Techniques: *MBE, XPS, SCS, simulation tools : NGSPICE*

Materials: *Si/Al/TiN/Y_2O_{3-x}/Pt stacks*

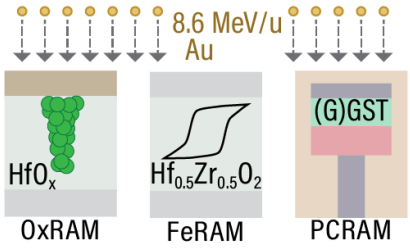
Abstract

This paper reports a material-oriented behavioural compact model for bipolar-type memristive devices. The model is written for the SPICE simulator and specifically deals with oxygen engineered yttrium oxide layers as the switching material. The model is able to represent not only the hysteretic I-V loop as many other memristor models do but, importantly, also its dependence on the oxygen content of the dielectric film. The starting point of our proposal is the dynamic memdiode model, which is modified appropriately so as to incorporate statistical information about the device electrical characteristics extracted from a large measurements database. In this way, the switching behaviour of the structures (low and high current states, set and reset voltages, etc.) as a function of the oxide stoichiometry can be tested before fabrication. A similar strategy can be applied to any other material-related fabrication parameter. Remarkably, this option opens up a new dimension for circuit designers.

OPERA Work Group

WG1 & WG2

Structural and Electrical Response of Emerging Memories Exposed to Heavy Ion Radiation



Reference: *ACS Nano 2022, 16, 9, 14463–14478;*
DOI: https://doi.org/10.1021/acsnano.2c04841

Authors: *T. Vogel, A.r Zintler, N. Kaiser, N. Guillaume, G. Lefèvre, M. Lederer, A. L. Serra, E. Piros, E. Kim, P. Schreyer, R. Winkler, D. Nasiou, R. R. Olivo, T. Ali, D. Lehninger, A. Arzumanov, C. Charpin-Nicolle, G. Bourgeois, L. Grenouillet, M.-C. Cyrille, G. Navarro, K. Seidel, T. Kämpfe, S. Petzold, C. Trautmann, L. Molina-Luna, and L. Alff*

Laboratories: *Institute of Materials Science, TU Darmstadt* ***(De)****, CEA LETI* ***(Fr)****, Fraunhofer IMPS, Center Nanoelectronic Technologies* ***(De)****, GSI Helmholtzzentrum für Schwerionenforschung* ***(De)***

Techniques: *MBE, XRD, HR-TEM, ACOM, ALD, P-V and I-V char., sputtering, heavy ion irradiation*

Materials: *HfO$_x$, HZO, GST, GGST*

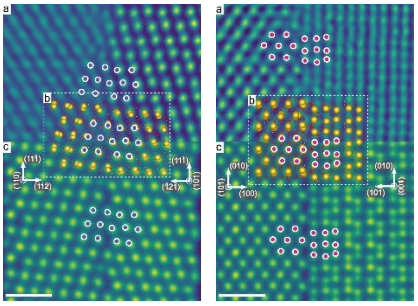
Abstract

Hafnium oxide- and GeSbTe-based functional layers are promising candidates in material systems for emerging memory technologies. They are also discussed as contenders for radiation-harsh environment applications. Testing the resilience against ion radiation is of high importance to identify materials that are feasible for future applications of emerging memory technologies like oxide-based, ferroelectric, and phase-change random-access memory. Induced changes of the crystalline and microscopic structure have to be considered as they are directly related to the memory states and failure mechanisms of the emerging memory technologies. Therefore, we present heavy ion irradiation-induced effects in emerging memories based on different memory materials, in particular, HfO$_2$-, HfZrO$_2$-, as well as GeSbTe-based thin films. This study reveals that the initial crystallinity, composition, and microstructure of the memory materials have a fundamental influence on their interaction with Au swift heavy ions. With this, we provide a test protocol for irradiation experiments of hafnium oxide- and GeSbTe-based emerging memories, combining structural investigations by X-ray diffraction on a macroscopic, scanning transmission electron microscopy on a microscopic scale, and electrical characterization of real devices. Such fundamental studies can be also of importance for future applications, considering the transition of digital to analog memories with a multitude of resistance states.

OPERA Work Group

WG1 & WG2

Controlling the Formation of Conductive Pathways in Memristive Devices



(11$\bar{1}$) and (020) textured HfO$_2$

Reference: *Advanced. Science 2022,9, 2201806*

DOI: 10.1002/advs.202201806

Authors: *R. Winkler, A. Zintler, S. Petzold, E. Piros, N. Kaiser, T. Vogel, D. Nasiou, K. P. McKenna, L. Molina-Luna, and L. Alff*

Laboratories: *Institute of Materials Science, TU Darmstadt* ***(De)***

Techniques: *MBE, sputtering, XRD, HR-TEM, FIB, DFT, Multislice Simulations*

Materials: *m-HfO$_2$ on c-Al$_2$O$_3$ and TiN*

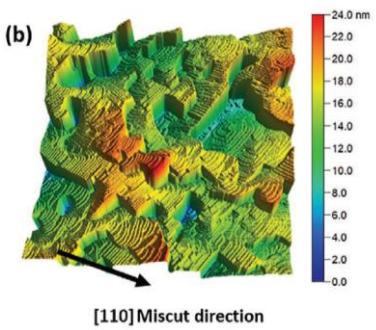
Abstract

Hafnium oxide plays an important role as a dielectric material in various thin-film electronic devices such as transistors and resistive or ferroelectric memory. The crystallographic and electronic structure of the hafnia layer often depends critically on its composition and defect structure. Here, we report two novel defect-stabilized polymorphs of substoichiometric HfO$_{2-x}$ with semiconducting properties that are of particular interest for resistive switching digital or analog memory devices. The thin-film samples are synthesized by molecular beam epitaxy with oxygen engineering that allows us to cover the whole range of metallic Hf with oxygen interstitials to HfO$_2$. The crystal and defect structures, in particular of a cubic low-temperature phase c-HfO$_{1.7}$ and a hexagonal phase hcp-HfO$_{0.7}$ are identified by X-ray diffraction, in vacuo electron spectroscopic, and transmission electron microscopic methods. With the help of UV/Vis transmission data, we propose a consistent band structure model for the whole oxidation range involving oxygen vacancy-induced in-gap defect states. Our comprehensive study of engineered hafnia thin films has an impact on the design of resistive memory devices and can be transferred to chemically similar suboxide systems.

OPERA Work Group

WG1 & WG2

Crystal Phase Control during Epitaxial Hybridization of III-V Semiconductors with Silicon



Abstract

The formation and propagation of anti-phase boundaries (APBs) in the epitaxial growth of III-V semiconductors on Silicon is still the subject of great debate, despite the impressive number of studies focusing on this topic in the last past decades. The control of the layer phase is of major importance for the future realization of photonic integrated circuits that include efficient light sources or for new nano-electronic devices, for example. Here, it is experimentally demonstrated that the main-phase domain overgrows the anti-phase domains (APDs) because it grows faster. A large-scale analysis of the phase evolution based on reflection high-energy electron diffraction and atomic force microscopy in the case of the molecular beam epitaxy of GaSb on Silicon (001) substrate is presented. The growth rate difference between the two domains is accurately measured and is shown to come from the atomic step distribution at the III-V surface. The influence of the substrate preparation as well as of the growth condition on this distribution is also clarified.

Reference: *Adv. Electron. Mater. 2022, 8, 2100777; DOI: 10.1002/aelm.202100777*

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

Laboratories: *IES (fr), Institut FOTON (fr), PDI (de), C2N (fr)*

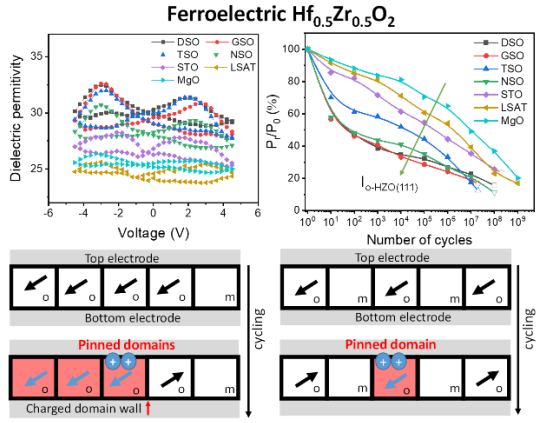
Techniques: *MBE, RHEED, AFM, TEM.*

Materials: *GaSb/Si(001), antiphase boundaries*

OPERA Work Group

WG1 & WG2

Positive Effect of Parasitic Monoclinic Phase of $Hf_{0.5}Zr_{0.5}O_2$ on Ferroelectric Endurance



Abstract

Endurance of ferroelectric HfO_2 needs to be enhanced for its use in commercial memories. Here, we investigate fatigue in epitaxial $Hf_{0.5}Zr_{0.5}O_2$ (HZO) instead of polycrystalline samples. Using different substrates, the relative amount of orthorhombic (ferroelectric) and monoclinic (paraelectric) phases is controlled. Epitaxial HZO films almost free of parasitic monoclinic phase suffer severe fatigue. In contrast, fatigue is mitigated in films with greater amount of paraelectric phase. This suggests that fatigue could be intrinsically pronounced in ferroelectric HZO. We argue that the enhancement of endurance in films showing coexisting phases results from the suppression of pinned domain propagation at ferroelectric-paraelectric grain boundaries, in contrast with rapid increase of the size of the pinned domains in single ferroelectric regions.

Reference: *Advanced Electronic Materials 2022, 8, 2100420; DOI: 10.1002/aelm.202100420*

Authors: *T. Song, S. Estandía, H. Tan, N. Dix, J. Gàzquez, I. Fina, and F. Sánchez*

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

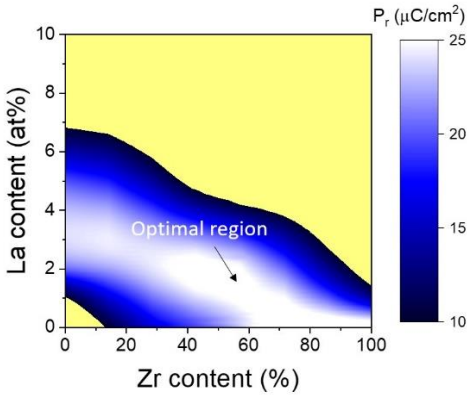
Techniques: *PLD, ferroelectric loops, endurance, polarization retention, dielectric constant, XRD, STEM*

Materials: *$Hf_{0.5}Zr_{0.5}O_2/La_{0.67}Sr_{0.33}MnO_3/SrTiO_3(001)$*

OPERA Work Group

WG1 & WG2

Ferroelectric $(Hf,Zr,La)O_2$ films



Reference: *Applied Materials Today 2022, 29, 101661; DOI: 10.1016/j.apmt.2022.101661*

Authors: *T. Song, S. Estandía, I. Fina, and F. Sánchez*

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

Techniques: *PLD, ferroelectric loops, dielectric constant, XRD, STEM*

Materials: *La doped HfO_2, ZrO_2 and $Hf_{0.5}Zr_{0.5}O_2$ films on $La_{0.67}Sr_{0.33}MnO_3/SrTiO_3(001)$*

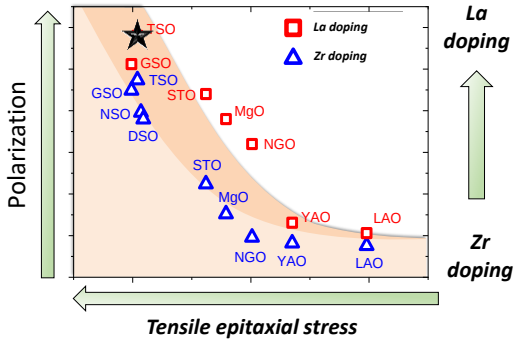
Abstract

The impact of La, Zr and Hf content on the crystal phases and ferroelectric and dielectric properties of $(Hf,Zr,La)O_2$ has been determined by investigating epitaxial films. The polarization of La-doped $Hf_{1-x}Zr_xO_2$ films strongly depends on La and Zr content, with remanent polarization ranging from 0 to about 30 μC/cm². The optimal La doping in $Hf_{1-x}Zr_xO_2$ increases from 0% to 2–5% for decreasing the Zr content from 100% (ZrO2) to 0% (HfO2). Structural characterization and dielectric permittivity measurements point to the correlation between crystal phases and polarization. In ZrO_2 films, an orthorhombic/tetragonal phase mixture likely evolves into a monoclinic/cubic/tetragonal phase mixture as La doping increases. In films with Hf content, when La content increases, the phases present in $Hf_{0.5}Zr_{0.5}O_2$ progressively evolve from orthorhombic and monoclinic to cubic, and in HfO_2 from monoclinic, to orthorhombic, and finally to cubic. This map of phases and polarization in the Hf-Zr-La oxide, established with epitaxial films, can be a model system for polycrystalline samples.

OPERA Work Group

WG1 & WG2

Synergetic contributions of chemical doping and epitaxial stress to polarization in ferroelectric HfO_2 films



Reference: *Applied Materials Today 2022, 29, 101621; DOI: 10.1016/j.apmt.2022.101621*

Authors: *T. Song, H. Tan, A.C. Robert, S. Estandía,, J. Gàzquez, F. Sánchez, and I. Fina*

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

Techniques: *PLD, ferroelectric loops, PFM, AFM, XRD, STEM*

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

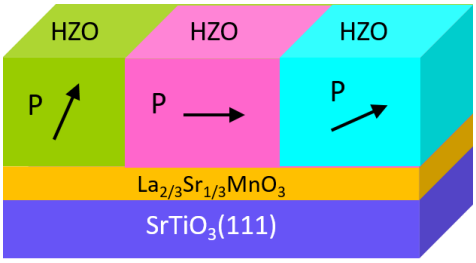
Abstract

Literature is rich on the study of different strategies to tailor ferroelectric properties of HfO_2. Among them, chemical doping is the most studied. La doped HfO_2 films have attracted interest because they show very low leakage current and high endurance. On the other hand, stress controlled by substrate selection has shown to induce ferroelectric properties variations in $Hf_{0.5}Zr_{0.5}O_2$ films. Here, we investigate stress effects in La-doped epitaxial HfO_2 films. Interestingly, ferroelectricity is measured in films grown on substrates having a broad range of lattice parameter from 3.71 to 4.21 Å. While comparing the obtained results with those obtained in epitaxial $Hf_{0.5}Zr_{0.5}O_2$, it is observed that La doped HfO_2 shows always larger remanent polarization (P_r) if the same substrate is used. Films grown on substrates with large lattice parameter ($TbScO_3$ and $GdScO_3$) show very large values of remanent polarization (29 μC/cm²), but it is also noticeable that the films on substrates with small parameter ($YAlO_3$) show remanent polarization above 5 μC/cm², whereas negligible P_r was detected in equivalent $Hf_{0.5}Zr_{0.5}O_2$ films. Therefore, chemical doping and epitaxial stress do not compete and can be both used to synergetically tailor ferroelectric properties and eventually improve them.

OPERA Work Group

WG1 & WG2

Ferroelectric $Hf_{0.5}Zr_{0.5}O_2$ films on $SrTiO_3(111)$



Reference: *J. Mater. Chem. C, 2022, 10, 8407;*
DOI: 10.1039/d2tc00996j

Authors: *T. Song, S. Estandía, N. Dix, J. Gàzquez, M. Gich, I. Fina, and F. Sánchez*

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

Techniques: *PLD, ferroelectric loops, endurance, polarization retention, XRD, STEM*

Materials: $Hf_{0.5}Zr_{0.5}O_2/La_{0.67}Sr_{0.33}MnO_3/SrTiO_3(111)$

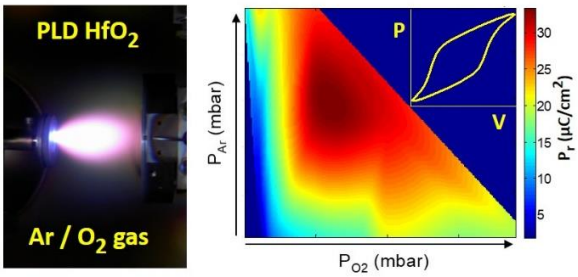
Abstract

Ferroelectric HfO_2 epitaxial films are of interest for determining intrinsic properties and for prototyping devices. Epitaxial (111)-oriented orthorhombic $Hf_{0.5}Zr_{0.5}O_2$ films grown on $La_{0.67}Sr_{0.33}MnO_3/SrTiO_3(001)$ are already being actively investigated. Presently, we have explored the use of $SrTiO_3(111)$ substrates. We show that the orthorhombic phase is stabilized by tilted epitaxy, and the orientation of orthorhombic crystallites is different from that of equivalent films on $SrTiO_3(001)$. The measured remanent polarization of above 14 $\mu C\ cm^{-2}$ agrees well with the expected value considering the crystal orientation, the fraction of the ferroelectric phase in the film, and the predicted polarization for ferroelectric HfO_2. High endurance and retention are also measured.

OPERA Work Group

WG1 & WG2

Large enhancement of ferroelectric polarization in $Hf_{0.5}Zr_{0.5}O_2$ films by low plasma energy pulsed laser deposition



Reference: *J. Mater. Chem. C, 2022, 10, 1084;*
DOI: 10.1039/d1tc05387f

Authors: *T. Song, R. Solanas, M. Qian, I. Fina, and F. Sánchez*

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

Techniques: *PLD, ferroelectric loops, XRD*

Materials: $Hf_{0.5}Zr_{0.5}O_2/La_{0.67}Sr_{0.33}MnO_3/SrTiO_3(001)$

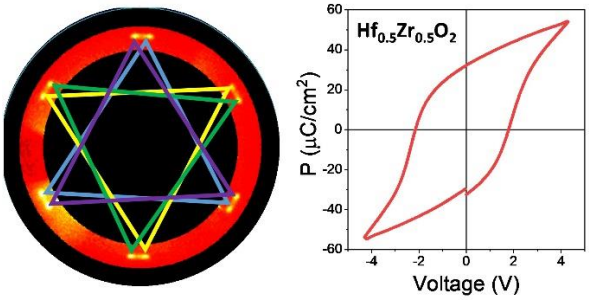
Abstract

The ferroelectric phase of HfO_2 is generally stabilized in polycrystalline films, which typically exhibit the highest polarization when deposited using low oxidizing conditions. In contrast, epitaxial film grown by pulsed laser deposition show low or suppressed polarization if low oxygen pressure is used. Epitaxial films are essential to better understand physical properties, and obtaining films that have intrinsic polarization is of great importance. In order to advance towards this objective, we have carried out a systematic study of the epitaxial growth of $Hf_{0.5}Zr_{0.5}O_2$ combining inert Ar gas with oxidizing O_2 gas. This allows us controlling the oxidizing conditions (through O_2 partial pressure) and the energy of the pulsed laser deposition plasma (through the total pressure of O_2 and Ar). A pressure of Ar high enough to significantly reduce plasma energy and low enough O_2 to reduce oxidation conditions is found to allow a large increase in ferroelectric polarization up to about 30 $\mu C\ cm^{-2}$, representing an increase of around 50% respect films grown by conventional pulsed laser deposition. This simple growth process, with high impact in the development of ferroelectric HfO_2, can be also beneficial in the growth of thin films of other materials by pulsed laser deposition.

OPERA Work Group

WG1 & WG2

Improved polarization and endurance in ferroelectric $Hf_{0.5}Zr_{0.5}O_2$ films on $SrTiO_3(110)$



Abstract

The metastable orthorhombic phase of $Hf_{0.5}Zr_{0.5}O_2$ (HZO) can be stabilized in thin films on $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) buffered (001)-oriented $SrTiO_3$ (STO) by intriguing epitaxy that results in (111)-HZO oriented growth and robust ferroelectric properties. Here, we show that the orthorhombic phase can also be epitaxially stabilized on LSMO/STO(110), presenting the same out-of-plane (111) orientation but a different distribution of the in-plane crystalline domains. The remanent polarization of HZO films with a thickness of less than 7 nm on LSMO/STO(110) is 33 $\mu C\ cm^{-3}$, which corresponds to a 50% improvement over equivalent films on LSMO/STO(001). Furthermore, HZO on LSMO/STO(110) presents higher endurance, switchable polarization is still observed up to 4×10^{10} cycles, and retention of more than 10 years. These results demonstrate that tuning the epitaxial growth of ferroelectric HfO_2, here using STO(110) substrates, allows the improvement of functional properties of relevance for memory applications.

Reference: *Nanoscale, 2022, 14, 2337;*
DOI: 10.1039/d1nr06983g

Authors: *T. Song, H. Tan, S. Estandía, J. Gàzquez, M. Gich, N. Dix, I. Fina, and F. Sánchez*

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

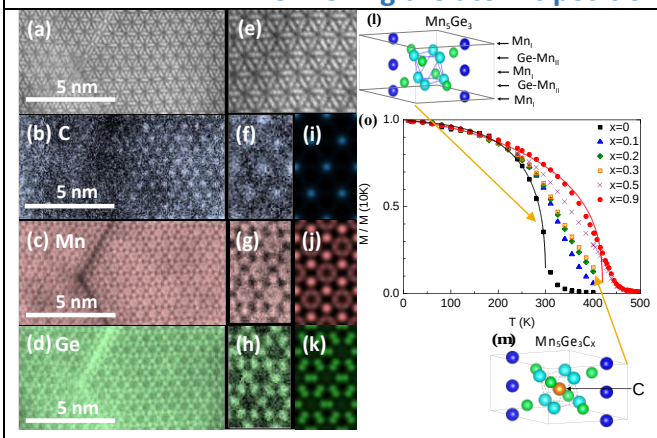
Techniques: *PLD, ferroelectric loops, endurance, polarization retention, PFM, XRD, STEM*

Materials: *$Hf_{0.5}Zr_{0.5}O_2/La_{0.67}Sr_{0.33}MnO_3/SrTiO_3(110)$*

OPERA Work Group

WG1 & WG2

Unveiling the atomic position of C in $Mn_5Ge_3C_x$ thin films



Abstract

We have used a combination of advanced techniques to extensively characterize the structural and magnetic properties of $Mn_5Ge_3C_x$ films grown on Ge(111) substrates by solid phase epitaxy (SPE) as a function of C concentration.
Heavily carbon-doped Mn_5Ge_3 (fig.(l and m)) is a unique compound for spintronics applications as it meets all the requirements for spin injection and detection in group-IV semiconductors. The carbon doping enhances the Curie temperature (T_C) up to 435 K (fig.(o)). However very little information is available on the $Mn_5Ge_3C_x$ structural properties and the genuine role played by C atoms.
In this work, the Mn and C chemical environments and positions in the Mn_5Ge_3 lattice have been thoroughly investigated using x-ray absorption spectroscopy techniques (x-ray absorption near-edge structures and extended x-ray absorption fine structures) and scanning transmission electronic microscopy (STEM, fig.(a)) combined to electron energy loss spectroscopy for the chemical analysis (fig.(b-h), simulations (i-k)). The results have been systematically compared to a variety of structures that were identified as favorable in terms of formation energy by ab initio calculations. For $x \leq 0.5$, the C atoms are mainly located in the octahedral voids formed by Mn atoms, which is confirmed by simulations and seen for the first time in real space by STEM. However, the latter reveals an inhomogeneous C incorporation, which is qualitatively correlated to the broad magnetic transition temperature. A higher C concentration leads to the formation of manganese carbide clusters that we identified as $Mn_{23}C_6$. Interestingly, other types of defects, such as interstitial Ge atoms, vacancies of Mn, and their association into line defects have been detected. They take part in the strain relaxation process and are likely to be intimately related to the growth process.

Reference: *Phys. Rev. Materials **6**, 074404 – Published 22 July 2022 - DOI:10.1103/PhysRevMaterials.6.074404*

Authors: *L.-A. Michez, M. Petit, V. Heresanu, V. Le Thanh, E. Prestat, F. d'Acapito, Q. Ramasse, F. Boscherini, P. Pochet, M. Jamet*

Laboratories: *CINaM **(Fr)**, University of Manchester **(GB)**, CNR-IOM-OGG c/o ESRF-LISA CRG **(Fr)**, SuperSTEM Laboratory **(GB)**, Department of Physics and Astronomy, Alma Mater Studiorum–Università di Bologna **(It)**, University Grenoble Alpes and CEA **(Fr)***

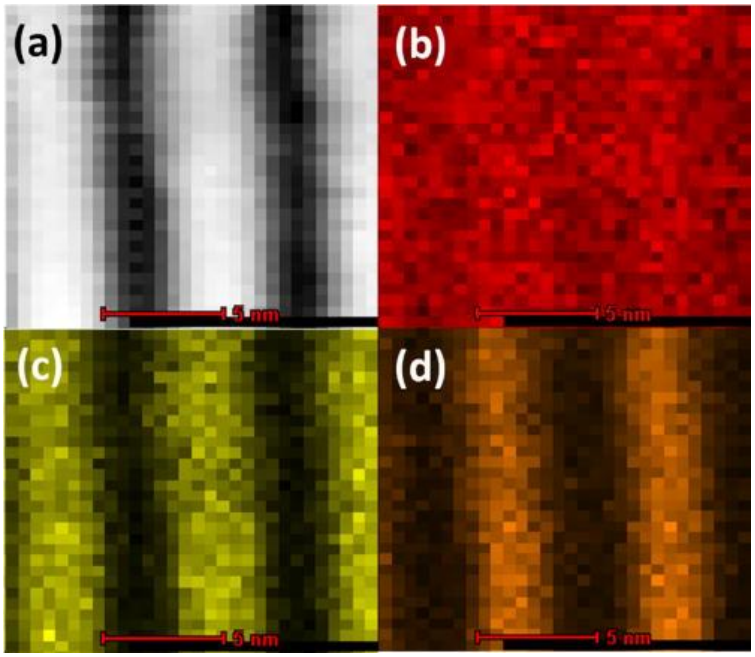
Techniques: *MBE, HAADF-STEM, STEM-EELS, EXAFS, XANES, SQUID-VSM, DFT*

Materials: *SiGe semiconductors, Mn_5Ge_3 ferromagnetic compound*

OPERA Work Group

WG1 & WG2

Pressure-dependent bandgap study of MBE grown {CdO/MgO} short period SLs using diamond anvil cell



Reference: *Appl. Phys. Lett.* 121, 242103 (2022)
https://doi.org/10.1063/5.0123342

Authors: A. Adhikari, P. Strak, P. Dluzewski, A. Kaminska, E. Przedziecka

Laboratories: Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, 02-668Warsaw, Poland

Techniques: *PA-MBE.*

Materials: *CdO/MgO Superlattices*

Abstract

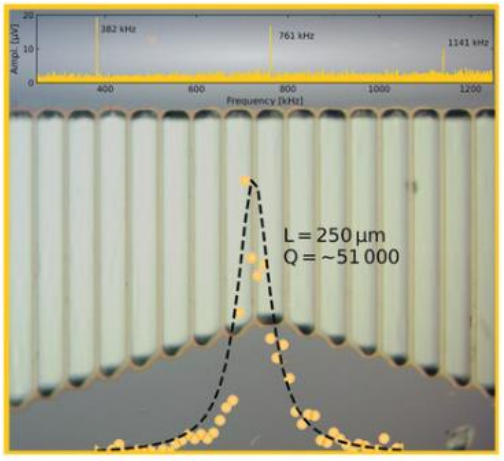
Semiconductor superlattices (SLs) have found widespread applications in electronic industries. In this work, a short-period SL structure composed of CdO and MgO layers was grown using a plasma-assisted molecular beam epitaxy technique. The optical property of the SLs was investigated by absorption measurement at room temperature. The ambient-pressure direct bandgap was found to be 2.76 eV. The pressure dependence of fundamental bandgap has been studied using a diamond anvil cell technique. It has been found that the band-to-band transition shifts toward higher energy with an applied pressure. The bandgap of SLs was varied from 2.76 to 2.87 eV with applied pressure varied from 0 to 5.9 GPa. The pressure coefficient for the direct bandgap of SLs was found to be 26 meV/GPa. The obtained experimental result was supported by theoretical results obtained using density functional theory calculations. The volume deformation potential was estimated using the empirical rule. We believe that our findings may provide valuable insight for a better understanding of {CdO/MgO} SLs toward their future applications in optoelectronics.

OPERA Work Group

WG1 and WG2

III- Applications-oriented material developments (WG2)

Stress Analysis and Q-Factor of Free-Standing (La,Sr)MnO3 Oxide Resonators



Abstract

High-sensitivity nanomechanical sensors are mostly based on silicon technology and related materials. The use of functional materials, such as complex oxides having strong interplay between structural, electronic, and magnetic properties, may open possibilities for developing new mechanical transduction schemes and for further enhancement of the device performances. The integration of these materials into micro/nano-electro-mechanical systems (MEMS/NEMS) is still at its very beginning and critical basic aspects related to the stress state and the quality factors of mechanical resonators made from epitaxial oxide thin films need to be investigated. Here, suspended micro-bridges are realized from single-crystal thin films of (La0.7,Sr0.3)MnO3 (LSMO), a prototypical complex oxide showing ferromagnetic ground state at room temperature. These devices are characterized in terms of resonance frequency, stress state, and Q-factor. LSMO resonators are highly stressed, with a maximum value of ≈260 MPa. The temperature dependence of their mechanical resonance is discussed considering both thermal strain and the temperature-dependent Young's modulus. The measured Q-factors reach few tens of thousands at room temperature, with indications of further improvements by optimizing the fabrication protocols. These results demonstrate that complex oxides are suitable to realize high Q-factor mechanical resonators, paving the way toward the development of full-oxide MEMS/NEMS sensors

Reference: *Small 2022, 18, 2202768;*
DOI: 10.1002/smll.202202768

Authors: *N. Manca, F. Remaggi, A. E. Plaza, L. Varbaro, C. Bernini, L. Pellegrino, D. Marré*

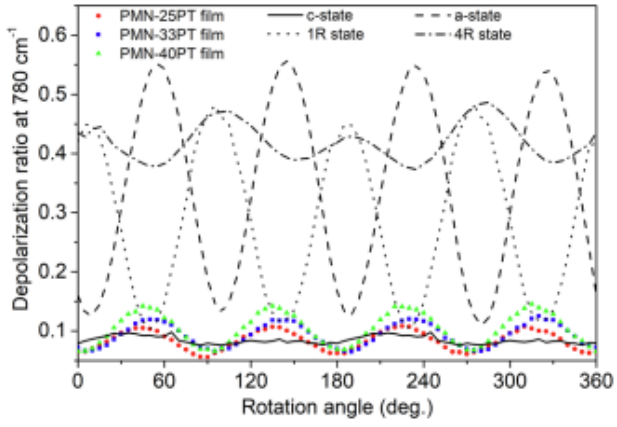
Laboratories: *CNR-SPIN **(It)**, Genoa Univ. **(It)***

Techniques: *PLD, optical lithography, mechanical & electrical measurements*

Materials: *(La,Sr)MnO3, SrTiO3*

OPERA Work Group
WG2

Polarization in pseudocubic epitaxial relaxed PMN-PT thin films



Abstract

Understanding the relationship between structural characteristics and functional properties of complex relaxor ferroelectric thin films is of high interest for designing materials with high performances. In this work, the structure of epitaxial relaxed pulsed-laser-deposited $Pb(Mg_{1/3}Nb_{2/3})O_3$-$xPbTiO_3$ (PMN-xPT; x = 25, 33, and 40) thin films on $LaNiO_3/SrTiO_3$ substrates is analyzed using a variety of diffraction and spectroscopic techniques. While based on the data obtained from high-resolution x-ray diffraction and scanning transmission electron microscopy analysis, the average structure of the PMN-xPT films is metrically cubic, micro-Raman polarimetry measurements indicate the tetragonal-like ferroelectric phase with marked preference for the polarization perpendicular to the film for all three compositions. The results of the Raman scattering analysis are supported by electromechanical properties of the samples, which clearly show that the films have a locally non-centrosymmetric structure. Furthermore, only a gradual enhancement of the electrical properties from PMN-25PT to PMN-40PT is observed, which is attributed to small tetragonal distortions that are highly similar for all three compositions.

Reference: *Appl. Phys. Lett. 120, 042901 (2022);*
DOI: 10.1063/5.0067531

Authors: *U. Trstenjak, N. Daneu, I. Rafalovskyi, J. Belhadi, D. Vengust, J. Hlinka and M. Spreitzer*

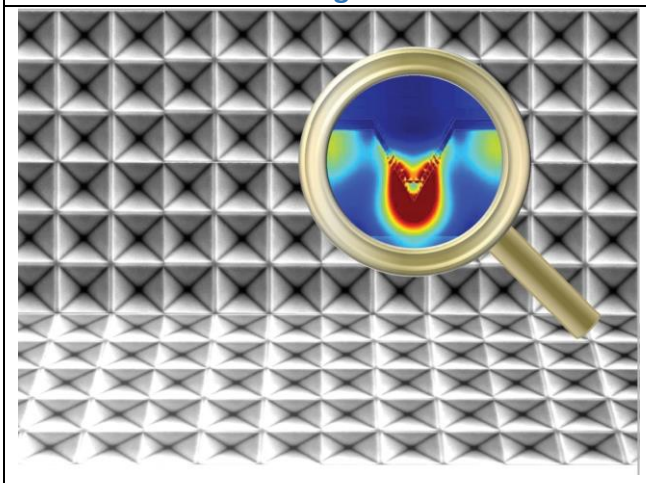
Laboratories: *JSI-K9 **(SI)**, FZU **(Cz)***

Techniques: *PLD, XRD (RSM), Raman, STEM, di-, ferro- and piezoelectric measurements*

Materials: *PMN-PT, LNO, STO*

OPERA Work Group
WG2

Efficient infrared sunlight absorbers based on gold-covered, inverted silicon pyramid arrays



Abstract

The transparency of silicon in the infrared region enables the design of nano/microstructures for implementation in devices to harvest the infrared (IR) part of the solar spectrum. Herein we report a strategy that uses arrays of inverted silicon pyramids covered with a thin gold film, which exhibit substantial light absorption in the infrared spectral range (below the gap of Si). The absorption stems from the resonant excitation at infrared wavelengths of surface-plasmon polaritons at the metal/dielectric interface mainly by tuning size and separation of the inverted pyramids. The array-parameter optimization proceeded by iteration of the calculation and measurement of the infrared response using finite difference time-domain simulations and Fourier-transform IR spectroscopy, respectively. We analyse the calculated near-field distributions specifically looking for the presence of hot spots, i.e. nano-sized regions of very high concentration of the electronic charge and strong electromagnetic field enhancement, and discuss their potential for hot-electron generation. We show two fabrication routes for this kind of metal/silicon metamaterial either by photolithography or scalable nanoimprint techniques for a seamless integration in optoelectronic fabrication processes.

Reference: *Materials Advances 3, 2364 (2022);*
DOI : 10.1039/D1MA01237A

Authors: *J. Hu, L. A. Pérez, J. L. García-Pomar, A. Mihi, M. Garriga, M. I. Alonso, and A. R. Goñi.*

Laboratories: *ICMAB-CSIC **(Es).***

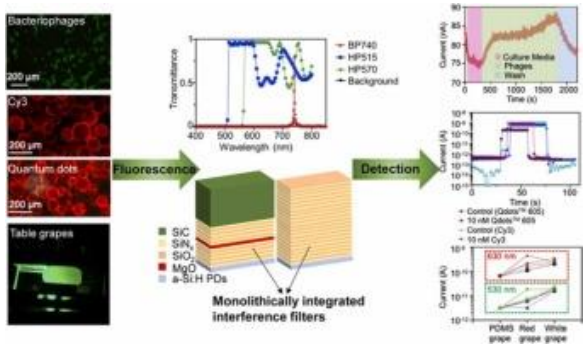
Techniques: *MBE, Lithography, Nanoimprinting, SEM, FDTD, FTIR*

Materials: *SiGe semiconductors, Au plasmonics*

OPERA Work Group

WG2

Monolithically integrated optical interference and absorption filters on thin film amorphous silicon photosensors for biological detection



Abstract

High selectivity of photosensors is needed for targeted biological detection. Optical interference filters are monolithically integrated with hydrogenated amorphous silicon thin film photosensors for fluorescence measurements in lab-on-chip applications using a methodology that enables customization of fluorescence detection for various applications. The design of the optical interference filters is tailored to match the requirements of each application and the filters are fabricated as nitride-oxide multilayers. The interference filters are combined with hydrogenated amorphous silicon-carbon alloys, which serve as long-pass absorption filters, depending on the spectral requirements. In this work we demonstrate the development of these filters, through simulations and design, followed by experimental fabrication and characterization of transmission spectra, and finally, integration with photosensors which are implemented in measurements to detect fluorescence in three different applications, including bacteriophage fluorescence, quantum dot and Cy3 fluorophores, and grape fluorescence for grape maturation monitoring, in a novel methodology that allows for simplification and greater portability of the measurement setup and negates the need to stack optical filters in fluorescence applications.

Reference: *Sensors and Actuators B-Chemical, Vol. 356, 131330 (2022)*
DOI: https://doi.org/10.1016/j.snb.2021.131330

Authors: *Nikolaidou, et.al*

Laboratories: *INESC MN **(Pt)**, Kaiserslautern University of Applied Sciences **(De)**, iMed. ULisboa **(Pt)**, INL **(Pt)**, University of Ljubljana - Laboratory of Photovoltaics and Optoelectronics **(Sl)**, Department of Chemical and Biological Engineering – IST **(Pt)***

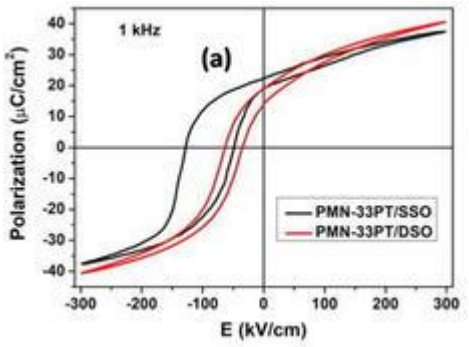
Techniques: *PECVD, Ion-beam deposition (IBD)*

Materials: *Thin-film amorphous silicon, silicon dioxide, silicon nitride, magnesium oxide*

OPERA Work Group

WG2

Large imprint in epitaxial $0.67Pb(Mg_{1/3}Nb_{2/3})O_3$-$0.33PbTiO_3$ thin films for piezoelectric energy harvesting applications



Abstract

Tuning and stabilizing a large imprint in epitaxial relaxor ferroelectric thin films is one of the key factors for designing micro-electromechanical devices with an enhanced figure of merit (FOM). In this work, epitaxial 500 nm-thick $0.67Pb(Mg_{1/3}Nb_{2/3})O_3$–$0.33PbTiO_3$ (PMN–33PT) films, free from secondary phases and with extremely low rocking curves (FWHM < 0.05°), are grown on $ScSmO_3$ (SSO) and $DyScO_3$ (DSO) substrates buffered with $SrRuO_3$ (SRO). The PMN–33PT is observed to grow coherently on SSO substrates (lattice mismatch of −0.7%), which is c-axis oriented and exhibits large tetragonality compared to bulk PMN–33PT, while on DSO substrates (lattice mismatch of −1.9%), the PMN–33PT film is almost completely relaxed and shows reduced tetragonality. Due to the compressive epitaxial strain, the fully strained PMN–33PT film displays typical ferroelectric P–E hysteresis loops, while the relaxed sample shows relaxor-like P–E loops. Samples present large negative imprints of about −88.50 and −49.25 kV/cm for PMN–33PT/SRO/SSO and PMN–33PT/SRO/DSO, respectively, which is more than threefold higher than the coercive field. The imprint is induced by the alignment of defect dipoles with the polarization and is tuned by the epitaxial strain. It permits the stabilization of a robust positive polarization state ($P_r \sim 20\ \mu C/cm^2$) and low dielectric permittivity (<700). In addition, the relaxed PMN–33PT film shows improved piezoelectric properties, with a 33% enhancement in $d_{33,eff}$ relative to the fully strained sample. The obtained low dielectric permittivity and the high piezoelectric coefficients at zero electric field in the studied PMN–33PT films hold great promise to maximize the FOM toward applications in piezoelectric devices.

Reference: *Appl. Phys. Lett. 121, 182903 (2022); DOI: 10.1063/5.0115777*

Authors: *J. Belhadi, Z. Hanani, U. Trstenjak, N.A. Shepelin, V. Bobnar, G. Koster, J. Hlinka, D. Pergolesi, T. Lippert, M. El Marssi and M. Spreitzer*

Laboratories: *JSI-K9* ***(SI)***, *FZU* ***(Cz)***, *PSI* ***(Ch)***, *UTwente* ***(NI)***

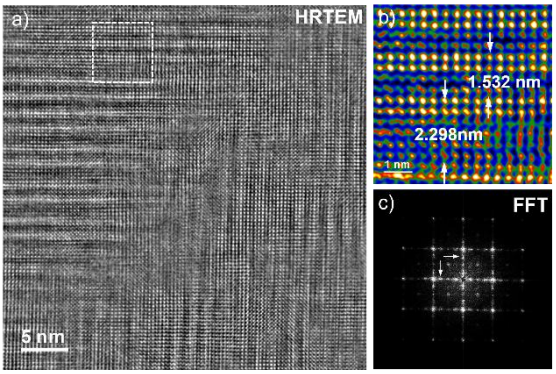
Techniques: *PLD, XRD (RSM), RHEED, di-, ferro- and piezoelectric measurements*

Materials: *PMN-PT, SRO, DSO, SSO*

OPERA Work Group

WG2

Evidence for antipolar displacements in $NaNbO_3$ thin films



Abstract

An antipolar phase is confirmed for $NaNbO_3$ thin films grown by pulsed laser deposition on $SrTiO_3$ (100) substrates. Reciprocal space maps and transmission electron microscopy reveal the presence of characteristic 1/4 superlattice reflections, indicative of the antipolar displacement of Na and Nb-ions. Furthermore, X-ray diffraction unveils the presence of two different orientations of the same phase for thin films beyond a critical thickness of about 60 nm. This orientation change with increasing thickness can be explained as an extraordinary strain compensation mechanism, changing magnitude and sign of the strain at the same time. The polarization vs electric field behavior exposes a characteristic thickness dependence, with the antiferroelectric phase stabilized for very thin films and a field induced ferroelectric hysteresis for a film of 310 nm having a maximum polarization of 26.5 $\mu C \cdot cm^{-2}$, which is among the highest values reported for $NaNbO_3$ thin films grown on $SrTiO_3$ (100).

Reference: *Appl. Phys. Lett. 121, 122906 (2022); DOI: 10.1063/5.0101739*

Authors: *T. Schneider, J. Cardoletti, H. Ding, M.-H. Zhang, T. Jiang, M. Major, P. Komissinskiy, L. Molina-Luna, and L. Alff*

Laboratories: *Institute of Materials Science, TU Darmstadt* ***(De)***

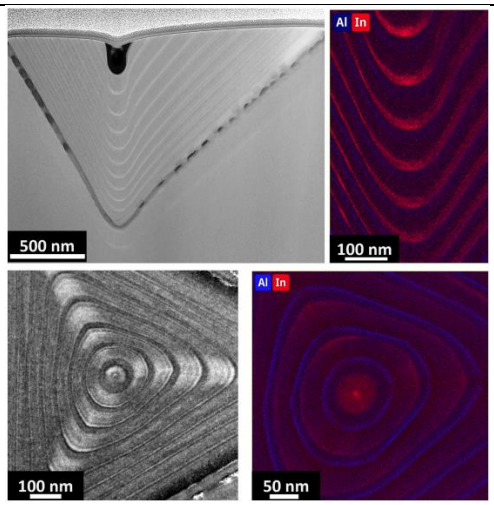
Techniques: *PLD, XRD, HR-TEM, P-E Measurement*

Materials: *$NaNbO_3$ and $LaNiO_3$ on $SrTiO_3$*

OPERA Work Group

WG2

Towards 3D characterisation of site-controlled InGaAs pyramidal QDs at the nanoscale



Reference: *Mater Sci 57, 16383–16396 (2022).*
DOI: 10.1007/s10853-022-07654-2

Authors: *K. M. Holsgrove, T. I. O'Reilly, S. Varo, A. Gocalinska, G. Juska, D. M. Kepaptsoglou, E. Pelucchi & M. Arredondo*

Laboratories: *Queen's University, Belfast,* ***(GB)***
University of Glasgow, ***(GB)****, Tyndall National Institute* ***(Ie)***
SuperSTEM Laboratory, ***(GB)****, University of York,* ***(GB)***

Techniques: *MOVPE, TEM, cleanroom processing*

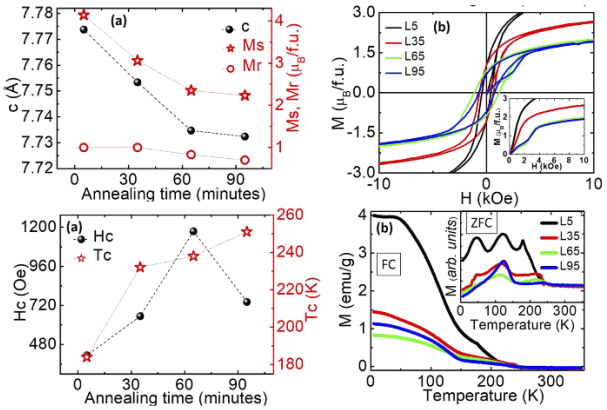
Materials: *(In(Al))GaAs (111)*

Abstract

In this work, we report an extensive investigation via transmission electron microscopy (TEM) techniques of InGaAs/GaAs pyramidal quantum dots (PQDs), a unique site-controlled family of quantum emitters that have proven to be excellent sources of single and entangled photons. The most striking features of this system, originating from their peculiar fabrication process, include their inherently 3-dimensional nature and their interconnection to a series of nanostructures that are formed alongside them, such as quantum wells and quantum wires. We present structural and chemical data from cross-sectional and plan view samples of both single and stacked PQDs structures. Our findings identify (i) the shape of the dot, being hexagonal and not triangular as previously assumed, (ii) the chemical distribution at the facets and QD area, displaying clear Indium diffusion, and (iii) a near absence of Aluminium (from the AlAs marker) at the bottom of the growth profile. Our results shed light on previously unreported structural and chemical features of PQDs, which is of extreme relevance for further development of this family of quantum emitters.

OPERA Work Group
WG2

Oxygen defect engineered magnetism of La_2NiMnO_6 thin films



Reference: *AIP Advances 12, 035116 (2022);*
DOI: 10.1063/9.0000360

Authors: *J. P. Palakkal, T. Schneider, and L. Alff*

Laboratories: *Institute of Materials Science, TU Darmstadt* ***(De)***

Techniques: *PLD, XRD, SQUID, HR-TEM, Transport*

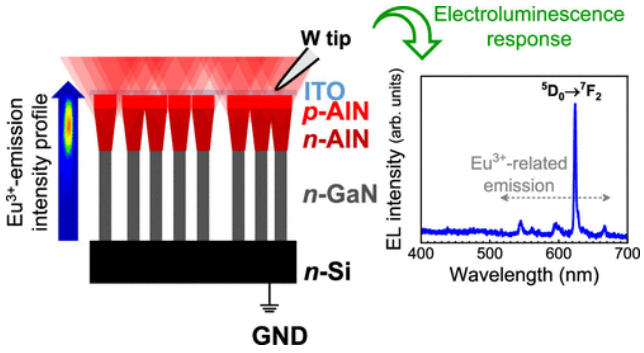
Materials: *La_2NiMnO_6 on $SrTiO_3$*

Abstract

The double perovskite La_2NiMnO_6 (LNMO) exhibits complex magnetism due to the competition of magnetic interactions that are strongly affected by structural and magnetic inhomogeneities. In this work, we study the effect of oxygen annealing on the structure and magnetism of epitaxial thin films grown by pulsed laser deposition. The key observations are that a longer annealing time leads to a reduction of saturation magnetization and an enhancement in the ferromagnetic transition temperature. We explain these results based upon epitaxial strain and oxygen defect engineering. The oxygen enrichment by annealing caused a decrease in the volume of the perovskite lattice. This increased the epitaxial strain of the films that are in-plane locked to the $SrTiO_3$ substrate. The enhanced strain caused a reduction in the saturation magnetization due to randomly distributed anti-site defects. The reduced oxygen defects concentration in the films due to the annealing in oxygen improved the ferromagnetic long-range interaction and caused an increase in the magnetic transition temperature.

OPERA Work Group
WG2

Europium-Implanted AlN Nanowires for Red Light-Emitting Diodes



Reference: *ACS Applied Nano Materials 5 (1), 972-984 (2022) DOI: https://doi.org/10.1021/acsanm.1c03654*

Authors: *Cardoso, J.; Correia, M.; Vermeersch, R.; Verheij, D.; Jacopin, G.; Pernot, J.; Monteiro, T.; Cardoso, S.; Lorenz, K.; Daudin, B.; Ben Sedrine, N.*

Laboratories: *Physics Department & i3N – Univ. Aveiro **(Pt)**, Univ. Grenoble Alpes – CEA **(Fr)**, Univ. Grenoble Alpes – CNRS **(Fr)**, IPFN **(Pt)**, INESC-MN **(Pt)**, i3N **(Pt)***

Techniques: *Molecular Beam Epitaxy, Ion Implantation, Rapid Thermal Annealing, Microfabrication, Optical Spectroscopy*

Materials: *Rare earth doped group-III nitrides, nanowires*

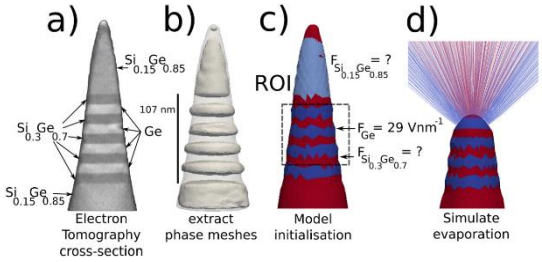
Abstract

Europium (Eu)-implanted AlN nanowire (NW) p–n junctions, subjected to rapid thermal annealing at 1000 °C, were investigated in view of application as red light-emitting diodes (LEDs). In a first step, the structural and optical properties of NWs implanted with two different fluences (1×10^{14} cm^{-2} and 5×10^{14} cm^{-2}) were studied. The luminescence of the trivalent Eu ions (Eu^{3+}) was achieved for both samples using below and above AlN bandgap energy excitation. The excitation below the AlN bandgap occurs through two broad bands, A1 (peaked at ~270 nm) and A2 (peaked at ~367 nm), associated with lattice defects. In addition to Eu^{3+} luminescence, other radiative channels linked to deep-level defects were identified in photoluminescence (PL). The cathodoluminescence (CL) relative intensity ratio between intra-ionic and defect-related emissions increases compared to that of PL. In both PL and CL, the Eu^{3+} luminescence intensity increases about three times for the highest fluence, while the contribution from radiative recombination at defects decreases. This study also allowed to map an in-depth profile of the optically active Eu^{3+}, revealing that it extends deeper than the range predicted by Monte Carlo simulations. Based on these findings, a proof-of-concept red LED is shown using the NWs implanted with the highest fluence. The devices exhibited the typical rectifying behavior of a p–n junction and an electroluminescence signal dominated by the $^5D_0 \rightarrow {}^7F_2$ transition (~624 nm) starting at a threshold voltage of 12 V. The demonstration of red LEDs based on Eu-implanted AlN NWs highlights the potential of such an approach for developing multi-color nano-emitters.

OPERA Work Group

WG2

Automated calibration of model-driven reconstructions in atom probe tomography



Reference: J. Phys. D: Appl. Phys. 55 (2022) 375301
DOI: 10.1088/1361-6463/ac7986

Authors: C. Fletcher, M. P Moody, C. Fleischmann, M. Dialameh , C. Porret, B. Geiser, and D. Haley

Laboratories: University of Oxford **(UK)**, imec **(Be)** KU Leuven **(Be)**, Cameca Instruments Inc. **(USA)**

Techniques: *RPCVD, APT, TEM*

Materials: *$Si_{0.15}Ge_{0.85}$ / 5x{Ge/$Si_{0.3}Ge_{0.7}$} $Si_{0.15}Ge_{0.85}$ and strained Ge / $Si_{0.3}Ge_{0.7}$ semiconductors*

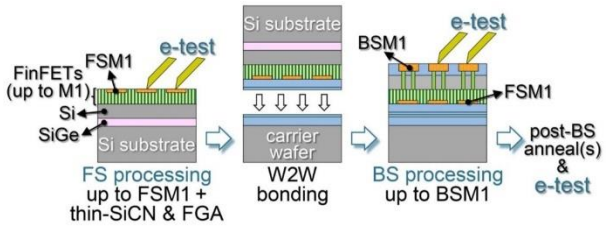
Abstract

Traditional reconstruction protocols in atom probe tomography frequently feature image distortions for multiphase materials, due to inaccurate geometric assumptions regarding specimen evolution. In this work, the authors' outline a new reconstruction protocol capable of correcting for many of these distortions. This new method uses predictions from a previously developed physical model for specimen field evaporation. The application of this new model-driven approach to both an experimental semiconductor multilayer system and a fin field-effect transistor device (finFET) is considered. In both systems, a significant reduction in multiphase image distortions when using this new algorithm is clearly demonstrated. By being able to quantitatively compare model predictions with experiment, such a method could also be applied to testing and validating new developments in field evaporation theory.

OPERA Work Group

WG2

Scaled FinFETs Connected by Using Both Wafer Sides for Routing via Buried Power Rails



Reference: *IEEE Transactions on Electron Devices*, vol. 69, no. 12, pp. 7173-7179, Dec. 2022,
Doi: 10.1109/TED.2022.3205561.

Authors: *A. Veloso, A. Jourdain, D. Radisic, R. Chen, G. Arutchelvan, B. O'Sullivan, H. Arimura, M. Stucchi, A. De Keersgieter, M. Hosseini, T. Hopf, K. D'have, S. Wang, E. Dupuy, G. Mannaert, K. Vandersmissen, S. Iacovo, P. Marien, S. Choudhury, F. Schleicher, F. Sebaai, Y. Oniki, X. Zhou, A. Gupta, T. Schram, B. Briggs, C. Lorant, E. Rosseel, A. Hikavyy, R. Loo, J. Geypen, D. Batuk, G. T. Martinez, J. P. Soulie, K. Devriendt, B. T. Chan, S. Demuynck, G. Hiblot, G. Van der Plas, J. Ryckaert, G. Beyer, E. Dentoni Litta, E. Beyne, and N. Horiguchi*

Laboratories: *Imec* ***(Be)***

Techniques: *RPCVD, TEM, FinFET, Buried Power Rail (BPR), Kelvin resistance, IV*

Materials: *Si/SiGe, SiGe:B, and Si:P semiconductors, Ti/TiN, W*

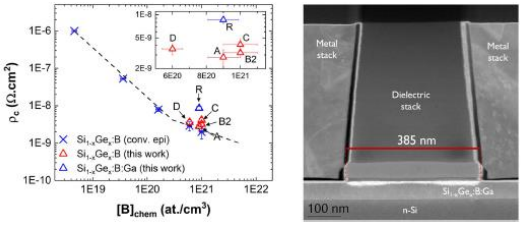
Abstract

We report on scaled finFETs built with a novel routing scheme wherein devices are connected via buried power rails (BPRs) from both wafer sides, with tight variability and matching control. On the wafer's frontside (FS), M1 lines (FSM1) are connected through V0 vias to M0A lines which are then linked to BPR lines by vias called VBPR while also contacting directly the device's S/D-epi. As for gate wiring, to enable in this work its access from both wafer sides, gate is also connected to BPR via V0 landing on it and on a neighboring M0A line set only on field-oxide. A single-step metallization for M0A and VBPR is preceded by in situ preclean(s) optimized for improved BPR-VBPR contact interface and R_{ext}, as confirmed electrically and by physical analysis. After FS processing, wafer flipping, bonding, and extreme thinning, highly scaled, ~323 nm deep nano-through-Si-vias (nTSVs) land on BPR, with tight overlay control and unchanged BPR resistance [26%–29% lower with improved tungsten (W)-fill], connecting them to the first backside (BS) metal level (BSM1). By moving the power delivery network to the BS (BSPDN), besides alleviating FS routing congestion, considerably smaller dynamic and static IR drop values are predicted from on-chip power heat maps generated for a low power 64-bit CPU at 2-nm design rules: 82% and 96% less worst-case values versus a reference configuration, respectively. P/NMOS show similar or even superior I_{ON}–I_{OFF} after BS processing and extra anneal(s) added for VT recovery, mobility and bias temperature instability (BTI) improvement—up to 8%/15% higher I_{ON} linked to anneal selection.

OPERA Work Group

WG2

B and Ga Co-Doped Si1–xGex for p-Type Source/Drain Contacts



Reference: *ECS Journal of Solid State Science and Technology 11, 024008, 2022,*
DOI: 10.1149/2162-8777/ac546e

Authors:

G. Rengo, C. Porret, A. Hikavyy, E. Rosseel, M. Ayyad, R.J.H. Morris, R. Khazaka, R. Loo, and A. Vantomme

Laboratories: *KU Leuven* ***(Be)****, imec* ***(Be)****, FWO* ***(Be)****, ASM Belgium* ***(Be)***

Techniques: *RPCVD, CTLM, SIMS, SEM, HR-XRD, XRR, m4pp, micro-Hall*

Materials: *SiGe:B, SiGe:B+Ga semiconductors*

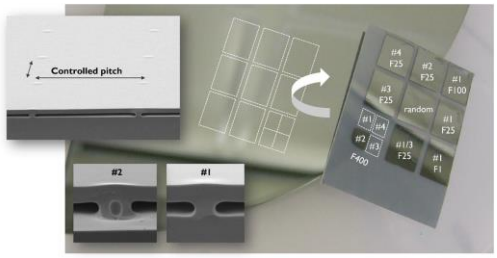
Abstract

Contact resistivity reduction at the source/drain contacts is one of the main requirements for the fabrication of future MOS devices. Current research focuses on methods to increase the active doping concentration near the contact region in silicon-germanium S/D epilayers. A possible approach consists in adding co-dopants during the epitaxy process. In the case of p-MOS, gallium can be used in addition to boron. In this work, the properties of in situ Ga and B co-doped $Si_{0.55}Ge_{0.45}$ layers are discussed. The surface morphologies, layer compositions, structural and electrical material properties are described and compared with those of a B-doped $Si_{0.55}Ge_{0.45}$ reference layer. Ga segregation occurring at the growth surface is evidenced. Post-epi surface cleans are required to obtain the correct Ga profiles in the $Si_{1-x}Ge_x$ layers from secondary ion mass spectrometry, otherwise altered by surface Ga knockon. The layer morphologies, crystalline quality and electrical properties show a progressive degradation with increasing Ga dose. Finally, specific titanium- $Si_{1-x}Ge_x$:B(:Ga) contact resistivity values have been extracted using the multi-ring circular transmission line method. The contact resistivity is lower for the Ga co-doped samples, the best contact properties (< 3 × 10^{-9} Ω.cm^2) being obtained for the sample grown with the lowest Ga-precursor flow.

OPERA Work Group

WG2

Wafer-scale Ge epitaxial foils grown at high growth rates and released from porous substrates for triple-junction solar cells



Reference: *Progress in Photovoltaics: Research and Applications, 1, 2022, DOI: 10.1002/pip.3634*

Authors: *V. Depauw, C. Porret, M. Moelants, E. Vecchio, K. Kennes, H. Han, R. Loo, J. Cho, G. Courtois, R. Kurstjens, K. Dessein, V. Orejuela, C. Sanchez-Perez, I. Rey-Stolle, I. García*

Laboratories: imec-imomec **(Be)**, University of Hasselt **(Be)**, imec, Leuven **(Be),** EnergyVille **(Be)**, Umicore Electro-Optic Materials **(Be)**, Universidad Politécnica de Madrid **(Es)**

Techniques: *RPCVD, MOCVD, RIE, litho, solar cell fabrication,* AFM, SIMS, SRP, ECCI, TEM, IV

Materials: *Ge, GaInP, GaInAs semiconductors*

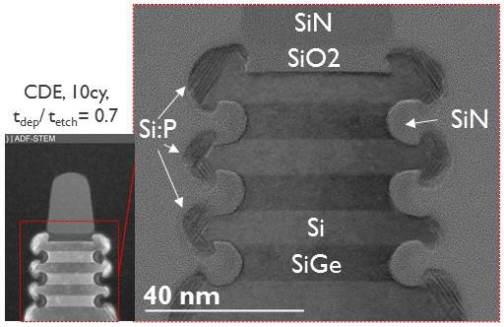
Abstract

Germanium is listed as a critical raw material, and for environmental and economic sustainability reasons, strategies for lower consumption must be implemented. A promising approach is Ge lift-off concepts, which enable to re-use the substrate multiple times. Our concept is based on the Ge-on-Nothing approach that is the controlled restructuring at high temperature of a macroporous Ge surface, forming a Ge foil weakly attached to its parent wafer. Its suitability as III–V epitaxy seed and support substrate has previously been demonstrated with proof-of-concept solar cells. This work focuses on bringing this concept to the next level, by upscaling the detachable area to a full 200-mm wafer scale, increasing foil thickness for sufficient light absorption in the Ge bottom cell, and improving the control on the strength that is bonding the suspended foil to its parent. By introducing a new high growth-rate epitaxy process from $GeCl_4$, and by engineering the GeON structure to introduce pillars with ad hoc density and shape, we fabricated P-type foils with tunable boron doping up to 15 µm in thickness and 11 cm x 11 cm in area, for which the detachment strength could be adapted to the stresses induced by the solar cell process steps. The surface roughness and the electrical and crystal qualities of these foils were inspected by AFM, SIMS, SRP, ECCI, and TEM to check the $GeCl_4$-based epitaxy conditions and to check that the ad hoc pillars were not introducing any damage. Small-area triple-junction lattice-matched GaInP/GaInAs/Ge solar cells were fabricated on 7-µm-thick Ge foils with various pillar densities and on a standard reference Ge wafer. The III–V layer nucleation was virtually the same on both substrates and the solar cells on the GeON foils performed in the same way as the cells on the Ge wafer, albeit a small loss in short-circuit current and open-circuit voltage that can be attributed to the thickness reduction and absence of rear-side passivation. We conclude that it is possible to gain control on the GeON detachability and upscale the concept to areas relevant for the space PV industry, proving that porous germanium is a serious candidate for replacement of bulk Ge wafers in view of a more sustainable multijunction solar cell process.

OPERA Work Group

WG2

Properties of Selectively Grown Si:P Layers below 500°C for Use in Stacked Nanosheet Devices



Reference: ECS Transactions, 109 (4) 93-98 (2022), DOI: 10.1149/10904.0093ecst

Authors: *E. Rosseel, C. Porret, A. Hikavyy, R. Loo, O. Richard, G. T. Martinez, D. Batuk, H. Mertens, E. Dentoni Litta, N. Horiguchi*

Laboratories: *Imec* ***(Be)***

Techniques: *RPCVD,* SEM, AFM, X-TEM, HRXRD, SIMS, m4pp, and micro-Hall Effect

Materials: *Si:P semiconductors*

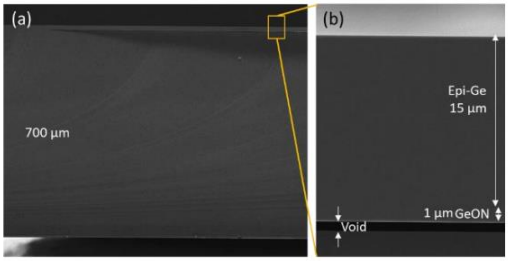
Abstract

We report on selectively grown Si:P layers below 500 ℃ targeting application in stacked nanosheet-based devices. In contrast to conventional approaches where selectivity is obtained at low temperatures using Cyclic-Deposition and Etch (CDE) with HCl/GeH_4 as an etchant, we rely for this work on Cl_2-based etching and the use of a higher order Si precursor which allows to maintain a high wafer throughput at low temperatures. We demonstrate that selective Si:P layers can be obtained with a resistivity below 0.3 mOhm.cm which can be grown selectively on fins and stacks with Si nanosheets.

OPERA Work Group

WG2

$GeCl_4$-based High Quality Ge epitaxy on Engineered Ge Substrates for Thin Multi-junction Solar Cells



Reference: *2022 IEEE 49th Photovoltaics Specialists Conference (PVSC)*, Philadelphia, PA, USA, 2022, pp. 0235-0238, doi: 10.1109/PVSC48317.2022.9938912.

Authors: *J. Cho, C. Porret, V. Depauw, G. Courtois, D. McDermott, R. Loo, K. Dessein, and R. Kurstjens*

Laboratories: *Umicore **(Be)**, Imec **(Be)***

Techniques: *RPCVD, SEM, AFM*

Materials: *Ge semiconductors*

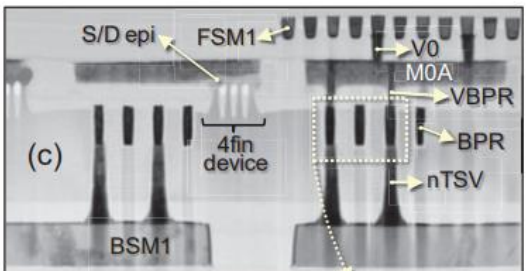
Abstract

Germanium, a critical raw material, is used as a template for III-V epitaxial growth and as a bottom cell in multijunction solar cells. To reduce the amount of germanium used, a detachable substrate is very interesting, especially if the Ge foil thickness can be adjusted as needed. In this study, the potential of $GeCl_4$-based epitaxy was demonstrated. A growth rate up to 190 nm/min and a thickness up to 15 µm were achieved. Detachable foils were then formed by porosification, annealing and epitaxial growth. The effective minority-carrier lifetime in the surfacepassivated foil could be measured and proved quite high: over 25 µs. Results presented in this contribution confirm that the soprepared foils constitute a suitable platform for the fabrication of high-performance multi-junction solar cells.

OPERA Work Group

WG2

Scaled FinFETs Connected by Using Both Wafer Sides for Routing via Buried Power Rails



Reference:

IEEE Symposium on VLSI Technology and Circuits (VLSI Technology and Circuits), Honolulu, HI, USA, 2022, pp. 284-285, doi: 10.1109/VLSITechnologyandCir46769.2022.9830177.

Authors: *A. Veloso, A. Jourdain, D. Radisic, R. Chen, G. Arutchelvan, B. O'Sullivan, H. Arimura, M. Stucchi, A. De Keersgieter, M. Hosseini, T. Hopf, K. D'have, S. Wang, E. Dupuy, G. Mannaert, K. Vandersmissen, S. Iacovo, P. Marien, S. Choudhury, F. Schleicher, F. Sebaai, Y. Oniki, X. Zhou, A. Gupta, T. Schram, B. Briggs, C. Lorant, E. Rosseel, A. Hikavyy, R. Loo, J. Geypen, D. Batuk, G. T. Martinez, J. P. Soulie, K. Devriendt, B. T. Chan, S. Demuynck, G. Hiblot, G. Van der Plas, J. Ryckaert, G. Beyer, E. Dentoni Litta, E. Beyne, and N. Horiguchi*

Laboratories: *Imec **(Be)***

Techniques: *RPCVD, TEM, FinFET, Buried Power Rail (BPR), Kelvin resistance, IV*

Materials: *Si/SiGe, SiGe:B, and Si:P semiconductors, Ti/TiN, W*

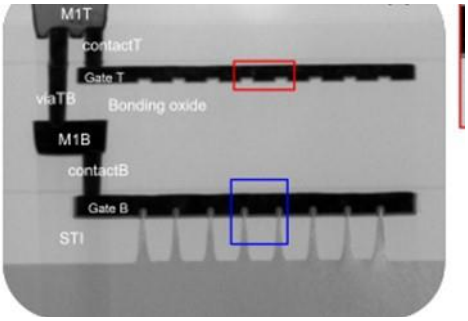
Abstract

We report on scaled finFETs with a novel routing scheme enabling connection via buried power rails (BPR) from both wafer sides, with tight variability/matching control. On the frontside (FS), contacting to p/n S/D-epi and BPR is done, after M0A and VBPR vias patterning, in a single metallization step with an optimized preclean reducing R ext while preserving a good BPR-VBPR contact interface. After wafer flipping, bonding and extreme thinning, highly scaled, ~323nm deep nano-through-Si-vias (nTSV) land on BPR, with tight overlay control and unchanged BPR resistance (26-29% lower with improved W-fill). By moving the power delivery network to the backside (BSPDN), besides alleviating routing congestion on the FS, considerably less dynamic and static IR drop values are predicted from on-chip power heat maps generated for a low power 64-bit CPU at 2nm design rules: 82% and 96% less (worst-case values) vs. a reference configuration, respectively. P/NMOS show similar or even superior I_{ON}-I_{OFF} after BS processing and extra anneal(s) added for V_T recovery, mobility and BTI improvement - up to 8/15% higher I_{ON} linked to anneal selection.

OPERA Work Group

WG2

Demonstration of 3D sequential FD-SOI on CMOS FinFET stacking featuring low temperature Si layer transfer and top tier device fabrication with tier interconnections



Reference: *2022 IEEE Symposium on VLSI Technology and Circuits (VLSI Technology and Circuits)*, Honolulu, HI, USA, 2022, pp. 330-331, doi: 10.1109/VLSITechnologyandCir46769.2022.9830400.

Authors: *A. Vandooren, N. Parihar, J. Franco, R. Loo, H. Arimura, R. Rodriguez, F. Sebaai, S. Iacovo, K. Vandersmissen, W. Li, G. Mannaert, D. Radisic, E. Rosseel, A. Hikavyy, A. Jourdain, O. Mourey, G. Gaudin, S. Reboh, L. Le Van-Jodin, G. Besnard, C. Roda Neve, B-Y. Nguyen, I. Radu, E. Dentoni Litta, N. Horiguchi*

Laboratories: *Imec **(Be)**, Soitec **(Fr)** CEA-Leti **(Fr)***

Techniques: *RPCVD, TEM, IV*

Materials: *Si, SiGe semiconductors, SOI,*

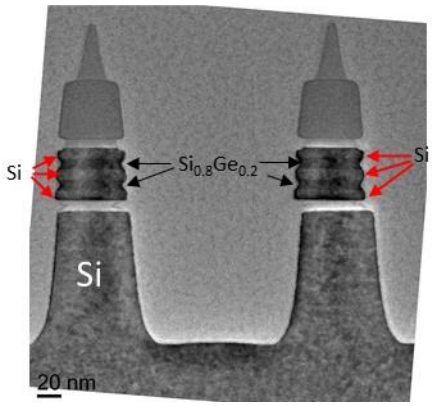
Abstract

3D sequential stacking is demonstrated using top tier FDSOI devices on bottom tier bulk finFETs. 3D integration and topbottom layer interconnectivity is validated through functional 3D via chains, 3D CMOS single inverters and inverter chain with transistors built in the top and bottom layers. Three different Si layer transfer flows, including a low temperature Smart CutTM, are investigated and compared electrically for top tier planar devices. Transfer of bi-axial tensile strained silicon is demonstrated with a 60-80% performance boost of the top tier nMOS device over the unstrained silicon devices. Further process optimization of the low temperature Smart CutTM transfer provided significant electron and hole mobility recovery of the top tier devices. Impact of the stacking on bottom tier finFET devices is also studied for various bottom gate stacks.

OPERA Work Group

WG2

Selective SiGe Vapor Etching Using Br2 in View of Nanosheet Device Isolation



Reference: *ECS Transactions, 109 (4) 135-140 (2022), DOI : 10.1149/10904.0135ecst*

Authors: *R. Loo, N. Gosset, M. Isaji, Y. I. Kawamura, A.Y.* Hikavyy, E. Rosseel, C. Porret, A. Nalin Mehta, and J.-M. Girard

Laboratories: *Imec **(Be)**, Air Liquide Laboratories, Innovation Campus **(Jpn)**, Air-Liquide Advanced Materials **(Fr)***

Techniques: *RPCVD, TEM, EDS, HR-XRD, AFM*

Materials: *Si/SiGe semiconductors,*

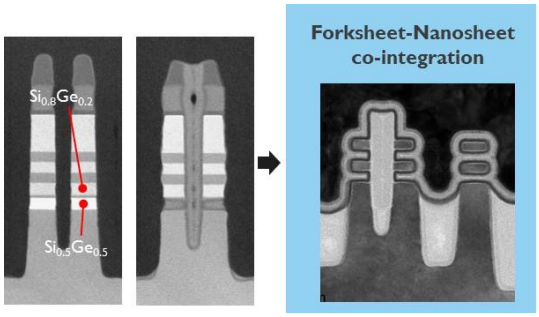
Abstract

Both forksheet and CFET device layouts contain local dielectric isolation layers to circumvent junction isolation trade-offs which are specific for these designs. Typical fabrication schemes start with the epitaxial growth of complicated SiGe/Si multi stacks with at least two different Ge concentrations where a Ge-rich SiGe layer is later replaced by an isolating dielectric. This work proposes a low temperature Br_2-based vapor etching process as an option for the selective SiGe removal in the isolation fabrication. After initial process screening on blanket epi layers to compare etching behavior for different process gases as function of material composition and crystallinity, it is demonstrated on patterned test structures that Br_2 etching enables high etching selectivity of $Si_{0.5}Ge_{0.5}$ towards Si and $Si_{1-x}Ge_x$ (x = 0.2 - 0.3).

OPERA Work Group

WG2

Forksheet FETs with Bottom Dielectric Isolation, Self-Aligned Gate Cut, and Isolation between Adjacent Source-Drain Structures



Reference: *2022 International Electron Devices Meeting (IEDM)*, San Francisco, CA, USA, 2022, pp. 23.1.1-23.1.4, Doi: 10.1109/IEDM45625.2022.10019497.

Authors: *H. Mertens, R. Ritzenthaler, Y. Oniki, P. Puttarame Gowda, G. Mannaert, F. Sebaai, A. Hikavyy, E. Rosseel, E. Dupuy, A. Peter, K. Vandersmissen, D. Radisic, B. Briggs, D. Batuk ,J. Geypen, G. Martinez-Alanis, F. Seidel, O. Richard, B.T. Chan, J. Mitard, E. Dentoni Litta, and N. Horiguchi*

Laboratories: *Imec* ***(Be)***

Techniques: *RPCVD, TEM, IV*

Materials: *Si/$Si_{0.8}Ge_{0.2}$/$Si_{0.5}Ge_{0.5}$, Si:P, SiGe:B semiconductors, BDI*

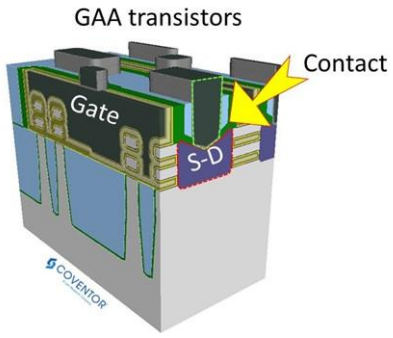
Abstract

We report on forksheet field-effect transistors that are isolated from the substrate by bottom dielectric isolation (BDI) formed by replacing a SiGe epitaxial layer with a dielectric film while the devices are anchored to the substrate by forksheet walls. Functional unipolar forksheet devices with BDI are demonstrated for both N- and PMOS, for wall widths down to 10 nm. In addition, we describe a scheme to isolate adjacent source-drain structures by the forksheet dielectric wall. This scheme relies on increasing wall height, by means of active area patterning hard mask engineering, to compensate for wall losses in downstream process modules. Finally, self-alignment of gate cut to active is demonstrated morphologically.

OPERA Work Group

WG2

Innovations in Transistor Architecture and Device Connectivity for Advanced Logic Scaling



Reference: *2022 International Conference on IC Design and Technology (ICICDT), Hanoi, Vietnam, 2022, pp. 51-54, Doi: 10.1109/ICICDT56182.2022.9933131.*

Authors: *A. Veloso, G. Eneman, A. De Keersgieter, P. Favia, A. Hikavyy, R. Chen, A. Jourdain, N. Horiguchi*

Laboratories: *Imec* ***(Be)***

Techniques: *RPCVD, NS-FETs, BPR, nTSV, SIMS, IV, TEM, NBD*

Materials: *Si/SiGe, SiGe:B, Si:P semiconductors*

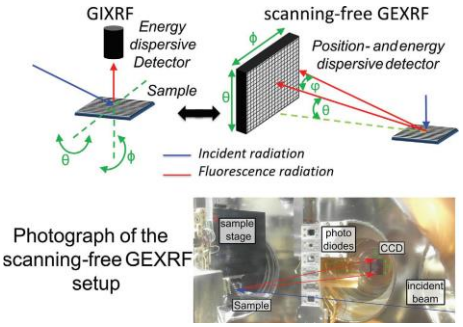
Abstract

We report on vertically stacked nanosheet (NS) FETs, focusing on the combined inner spacers and source/drain (S/D) epitaxial growth modules sequence, a key integration flow differentiator as compared to finFETs, addressing the impact and control of parasitics and channel strain engineering. The use of both wafer sides for device connection, via nTSVs landing on buried power rails (BPR) after extreme wafer thinning, is also discussed. This configuration is shown to be advantageous for obtaining reduced IR drop values and for, overall, enabling enhanced performance and additional area scaling. It also has the potential to further expand such as to include extra options, together with novel devices/circuits and for various applications.

OPERA Work Group

WG2

Simultaneous Dimensional and Analytical Characterization of Ordered Nanostructures



Reference: *Small 18 (6), 2105776, 2022*
DOI: 10.1002/smll.202105776

Authors: *P. Hönicke, Y. Kayser, K.V. Nikolaev, V. Soltwisch, J.E. Scheerder, C. Fleischmann, T. Siefke, A. Andrle, G. Gwalt, F. Siewert, J. Davis, M. Huth, A. Veloso, R. Loo, D. Skroblin, M. Steinert, A. Undisz, M. Rettenmayr, and B. Beckhoff B*

Laboratories: *PTB **(De)**, NRC Kurchatov Institute **(Ru)**, imec **(Be)**, KU Leuven **(Be)**, Friedrich Schiller University Jena **(De)**, HZB **(De)**, EOS **(De)**, PNDetector **(De)**, TU Chemnitz **(De)***

Techniques: *RPCVD, Ion Beam Sputtering, EBL, scanning-free GEXRF, GIXRF, AFM, TEM, SEM*

Materials: *SiGe semiconductors,* TiO2-HfO2

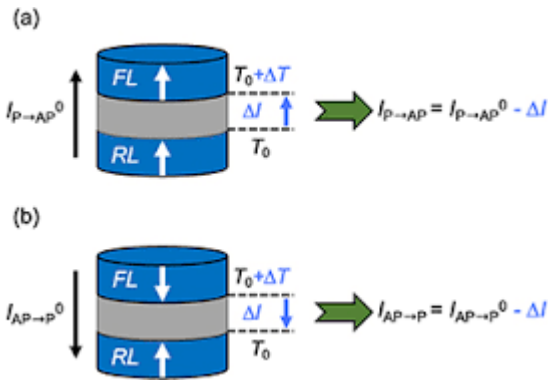
Abstract

The spatial and compositional complexity of 3D structures employed in today's nanotechnologies has developed to a level at which the requirements for process development and control can no longer fully be met by existing metrology techniques. For instance, buried parts in stratified nanostructures, which are often crucial for device functionality, can only be probed in a destructive manner in few locations as many existing nondestructive techniques only probe the objects surfaces. Here, it is demonstrated that grazing exit X-ray fluorescence can simultaneously characterize an ensemble of regularly ordered nanostructures simultaneously with respect to their dimensional properties and their elemental composition. This technique is nondestructive and compatible to typically sized test fields, allowing the same array of structures to be studied by other techniques. For crucial parameters, the technique provides sub-nm discrimination capabilities and it does not require access-limited large-scale research facilities as it is compatible to laboratory-scale instrumentation.

OPERA Work Group

WG2

Seebeck effect and Joule heating in CoFeB/MgO/CoFeB-based perpendicular magnetic tunnel junctions with low resistance area product



Reference: *J.Phys.D, 55, 265302 (2022),*
DOI: https://doi.org/10.1088/1361-6463/ac5e8a

Authors: *Lv, J. Fidalgo, T. Kampfe, S. Riedel, J. Langer, J. Wrona, O. Berthold, P. P. Freitas, and S. Cardoso*

Laboratories: *INESC MN **(Pt)**, IST **(Pt)**, Fraunhofer Institute for Photonic Microsystems IPMS **(De)**, Singulus Technologies AG **(De)***

Techniques: *Magnetron sputtering, magnetic annealing, nanofabrication, e-beam lithography*

Materials *Epitaxial MgO/CoFeB thin films, thin films with perpendicular anisotropy magnetization*

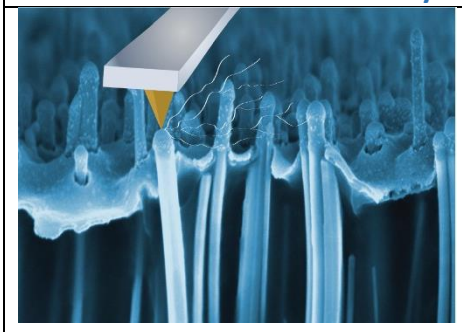
Abstract

Perpendicular magnetic tunnel junctions (p-MTJs) have attracted great interest due to their excellent performance in spin-transfer-torque magnetic random access memories (STT-MRAMs). Here, the resistance states can be manipulated by an applied current in the order of 109–1010 A m−2, yet the appearance of a heating influence must be understood. In this work, we systematically study the Seebeck effect in nano scale p-MTJs induced due to Joule heating by the tunneling current. The CoFeB/MgO/CoFeB-based p-MTJs were nanofabricated and the current-induced switching was characterized. We find a sign change of the thermovoltage (ΔV) between AP (positive) and P (negative) states, indicating a significant dependence of the Seebeck effect on the magnetic state of the p-MTJ. The temperature distribution in the stack was simulated, by which the Seebeck coefficient (S) and the tunnel magneto-Seebeck ratio were calculated. Our further study indicates that the thermal STT can reduce the switching currents, showing the possibility to re-use this dissipative heating energy. To improve the efficiency of the energy re-use, a method is proposed through the materials optimization of the non-magnetic layers but still retaining high tunneling magnetoresistance effect. Our study shows that the magneto-Seebeck effect plays an important role in the p-MTJs, which can be crucial and must be considered in the design of the high performance p-STT-MRAMs and thermal-assisted MRAMs.

OPERA Work Group

WG2

Electromechanical conversion efficiency of GaN NWs: critical influence of the NW stiffness, the Schottky nano-contact and the surface charge effects



Abstract

The piezoelectric nanowires (NWs) are considered as promising nanomaterials to develop high-efficient piezoelectric generators. Establishing the relationship between their characteristics and their piezoelectric conversion properties is now essential to further improve the devices. However, due to their nanoscale dimensions, the NWs are characterized by new properties that are challenging to investigate. Here, we use an advanced nano-characterization tool derived from AFM to quantify the piezo-conversion properties of NWs axially compressed with a well-controlled applied force. This unique technique allows to establish the direct relation between the output signal generation and the NW stiffness and to quantify the electromechanical coupling coefficient of GaN NWs, which can reach up to 43.4%. We highlight that this coefficient is affected by the formation of the Schottky nano-contact harvesting the piezo-generated energy, and is extremely sensitive to the surface charge effects, strongly pronounced in sub-100 nm wide GaN NWs. These results constitute a new building block in the improvement of NW-based nanogenerator devices.

Reference: *Nanoscale, 2022,14, 4965; doi.org/10.1039/D1NR07863A*

Authors: *N. Gogneau, P. Chrétien, T. Sodhi, L. Couraud, L. Leroy, L. Travers, J-C Harmand, F. H. Julien, M. Tchernycheva, F.C Houzé*

Laboratories: *C2N **(Fr)** ; GEEPS **(Fr)**.*

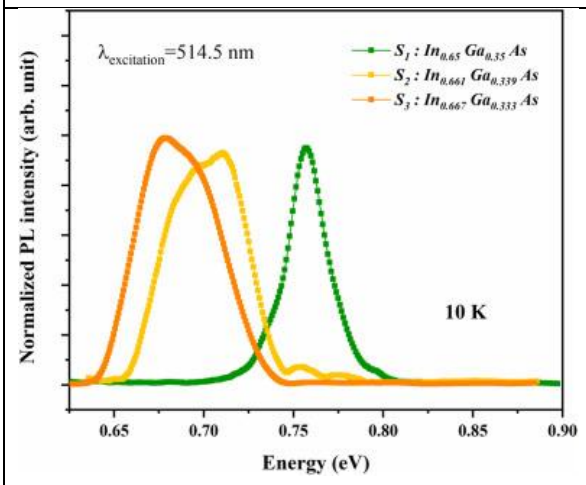
Techniques: *PA-MBE, AFM.*

Materials: *GaN Nanowires.*

OPERA Work Group

WG2

Theoretical analyses of the carrier localization effect on the photoluminescence of In-rich InGaAs layer grown on InP



Abstract

The free buffer InGaAs/InP structure has been elaborated by Metal Organic Vapor Phase Epitaxy (MOVPE). High indium content is chosen to reduce the bandgap energy of the ternary material with direct bandgap to be promoted for Infrared optoelectronic devices. In this work, the temperature dependent photoluminescence (TDPL) analysis of In-rich InxGa1−xAs (x = 0.65: S1, x = 0.661: S2, and x = 0.667 S3) samples are of the central focus. The S-shaped behavior recorded at low temperature range in the III-V ternary is quantitatively studied herein by Localized State Ensemble (LSE) model. A comparison between the semi-empirical evolution of luminescence versus temperature and our numerical simulation proves the adequacy of computational details, used in LSE model, in well reproducing the S-shape feature. The numerical simulation well matched with PL spectra proving that the localization phenomenon is stronger when increasing the Indium mole fraction. The clustering effect in In-rich structure seems to be beneficial for enhancing the carrier localization within InxGa1−xAs by localizing carriers from away extended defects that behave probably as non- radiative centers. This is indicative of the utmost importance of localization phenomenon in trapping carriers within localized states instead of dislocations and defects, owing to clustering of indium atoms.

Reference: *Materials Science in Semiconductor Processing, 140, 106411. (2022). DOI: 10.1016/j.mssp.2021.106411*

Authors: *Arbia, M. B., Smiri, B., Demir, I., Saidi, F., Altuntas, I.,Hassen, F., and Maaref, H.*

Laboratories: *The Nanophotonics Research and Application Center at Sivas Cumhuriyet University (CUNAM) (Tr), Laboratory of Micro-optoelectronics and Nanostructures (LMON) at University of Monastir (Tn)*

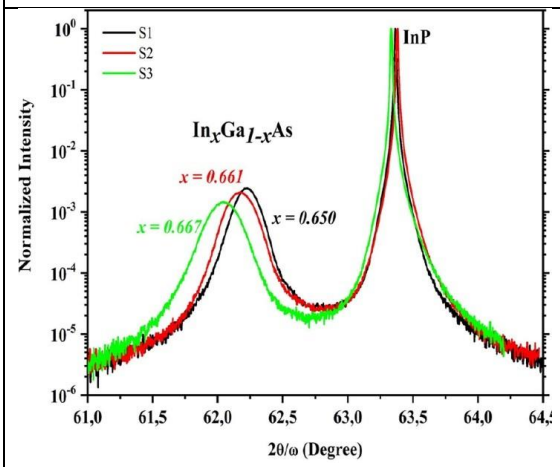
Techniques: *MOVPE, PL*

Materials: *InGaAs/InP*

OPERA Work Group

WG2

Systematic optical study of high-x InxGa1-xAs/InP structures for infrared photodetector applications



Reference: *Optics and Laser Technology, 148, 107714. (2022); DOI: 10.1016/j.optlastec.2021.107714*

Authors: *Badreddine S, Joshya RS, Ilkay D, Faouzi S, Ismail A, Lagarde D, Rober C, Xavier M, and Hassen M.*

Laboratories: *The Nanophotonics Research and Application Center at Sivas Cumhuriyet University (CUNAM) (Tr), Laboratory of Micro-optoelectronics and Nanostructures (LMON) University of Monastir (Tn), and INSACNRS-UPS, LPCNO at the University of Toulouse (Fr)*

Techniques: *HR-XRD, PR, PL, and TRPL Spectroscopy*

Materials: *InGaAs/InP*

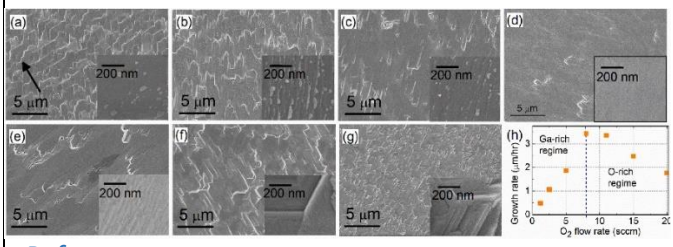
Abstract

Optical and structural properties in high-x InxGa1-xAs (x > 0.65) samples with varying indium concentration grown on InP (100) substrate are reported. By increasing the indium fraction, it was found by the high-resolution X-ray diffraction (HR-XRD) study that the dislocation density in the InxGa1-xAs epitaxial layer significantly increased, and the surface quality deteriorated remarkably. Photoreflectance (PR) spectra show the presence of Franz-Keldysh Oscillations (FKOs) features above the InxGa1-xAs energy bandgap. The strain-induced electric field is then estimated directly from the FKOs periods. Temperature-dependent photoluminescence (TDPL) measurements from 10 K to 300 K showed carrier locations (S-shape). This abnormal behavior is due to the dislocation density associated with fluctuations in the indium concentration. A quasi-stationary rate equation model for the temperature-dependent luminescence spectra of the localized state material system is proposed to interpret the band gap emission process quantitatively. Low-temperature (10 K) time-resolved PL measurements show the increase of lifetime with increasing the indium concentration. Yet, the addition of only 1.7% of indium concentration results in a strong enhancement of PL lifetime by ~ 80%. All these results reveal a more precise picture of the localization and recombination mechanisms of photogenerated carriers in the InGaAs layer, which could be the crucial factors in controlling the performance of high indium content InGaAs SWIR detector

OPERA Work Group

WG2

Close oxygen coupled low-pressure chemical vapor deposition growth of high quality β–Ga2O3 on sapphire



Reference: *Materials Science in Semiconductor Processing 146 (2022): 106645; DOI: 10.1016/j.mssp.2022.106645*

Authors: *Akyol F, and Demir İ.*

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

Techniques: *close oxygen coupled LPCVD, Field emission scanning electron microscopy (FESEM), AFM, and HRXRD*

Materials: *Ga_2O_3*

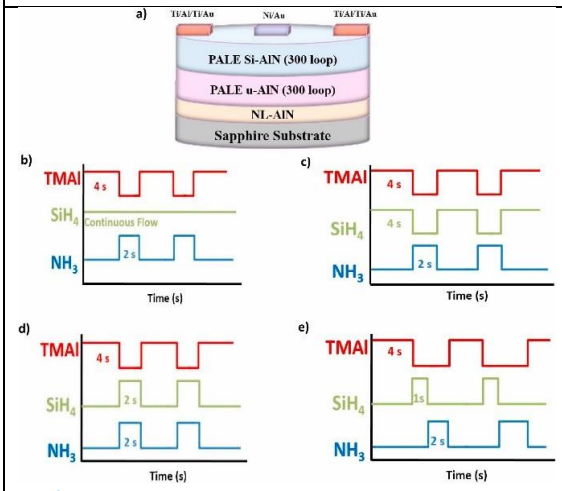
Abstract

We report on the close oxygen coupled low-pressure chemical vapor deposition (COC-LPCVD) hetero-epitaxial growth of atomically smooth (−201) oriented β −Ga_2O_3 on c-plane sapphire. Utilizing a dedicated line within the main tube, O_2 could be delivered to the substrate surface which enables effective control of growth regime. Under optimized conditions (Ga-rich and near stoichiometric feed rate), step flow growth was obtained with X-ray rocking curve full-width at half maximum of 0.09° and 0.20° at a growth rate of 0.49 μm/h and 3.42 μm/h, respectively. On the other hand, oxygen-rich growth at high growth rates produced in-plane rotational domains. In addition, the alignment of single crystal (−201) β − Ga_2O_3 with respect to the sapphire offcut direction was revealed such that [-20-1] β−Ga_2O_3 is along [11−20] (offcut direction) sapphire. This study demonstrates the potential of the versatile COC-LPCVD system on the thin film growth of high quality β − Ga_2O_3.

OPERA Work Group

WG2

Growth and characterization of PALE Si-doped AlN on sapphire substrate by MOVPE



Abstract

In this study, we report different SiH4 flow condition effects on crystal, surface, optical, and electrical characteristics of heteroepitaxial Metal-Organic Vapor Phase Epitaxy (MOVPE) grown AlN layers on sapphire substrates. Adjustment of growth kinetics is very important to control the doping. Therefore, pulsed atomic layer epitaxy (PALE) was used to control the growth kinetics and reduce parasitic reactions that inevitably caused adverse impact on the properties of the epitaxial AlN films. As a result of HRXRD (high resolution x-ray diffraction) analysis, the (002) ω FWHM decreased significantly with the PALE method, while the increase occurred due to the development of V defects for the (102) ω scan. Atomic force microscopy (AFM) analyzes showed that SiH4 led to a 3D-like growth mode. It was demonstrated that the increased SiH4 flow increased Si incorporation into the Si-doped AlN layer while increased the sheet resistance due to the self-compensating effect obtained from secondary ion mass spectroscopy (SIMS) and I–V measurement results.

Reference: *Materials Science in Semiconductor Processing, 142, 106464. (2022); DOI: 10.1016/j.mssp.2022.106464*

Authors: *Pürlü KM, Kocak MN, Yolcu G, Perkitel I, Altuntaş İ, Demir I.*

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

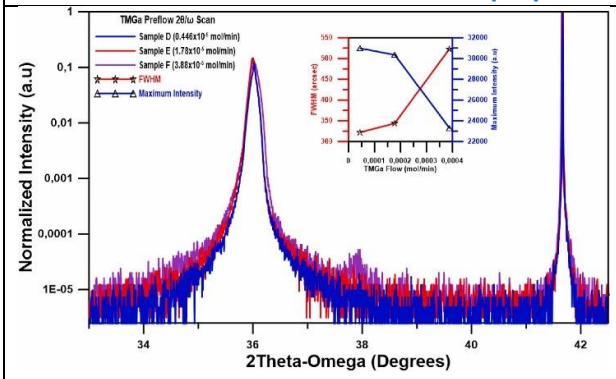
Techniques: *MOVPE, HRXRD, AFM, SIMS, UV-VIS-NIR Spectrophotometer, and Raman*

Materials: *AlN/Sapphire*

OPERA Work Group

WG2

The influence of TMGa pre-flow time and amount as surfactant on the structural and optical properties of AlN epilayer



Abstract

AlN is used as a template layer for deep UV (DUV) emitter and detector applications, because of its wide bandgap and high thermal conductivity. In this study, trimethylgallium (TMGa) source is used as surfactant to improve crystal quality and decrease dislocation density (DD) of AlN layers grown on sapphire (Al_2O_3) substrate surfaces by Metal Organic Vapor Phase Epitaxy (MOVPE) system. TMGa pre-flow time and pre- flow amount that TMGa pre-flow to the nucleation stage are the subjects of two distinct optimization studies. The structural and optical properties of grown AlN are examined by a high-resolution X-ray diffractometer (HR-XRD), Raman spectroscopy, and UV–Vis–NIR spectrophotometer, respectively. TMGa pre-flow time and TMGa pre-flow amount determined to obtain high crystal quality AlN epilayers are 2 s and 0.446 × 10^{-5} mol/min, respectively. HR-XRD investigation of these growths yields FWHM values of 159/2718 arcsec and 201/1550 arcsec for the ω (002) and ω (102) scans, respectively.

Reference: *Micro and Nanostructures, 168, 207301 (2022); DOI: 10.1016/j.micrna.2022.207301*

Authors: *Yolcu G, Simsek I, Kekul R, Altuntas I, Horoz S, and Demir I.**

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

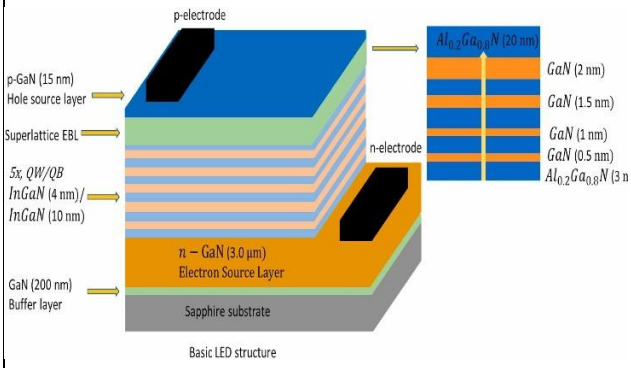
Techniques: *MOVPE, HR-XRD, Raman spectroscopy and UV- VIS-NIR Spectrophotometer*

Materials: *AlN/Sapphire*

OPERA Work Group

WG2

Sensitivity of indium molar fraction in InGaN quantum wells for near-UV light-emitting diodes



Reference: *Micro and Nanostructures 165 (2022): 207208.; DOI: 10.1016/j.micrna.2022.207208*

Authors: *Sharif MN, Wali Q, ur Rehman H, Xing Z, Khan SU, Zhang A, Demir I, Wang F, and Liu Y.*

Laboratories: *The Nanophotonics Research and Application Center at Sivas Cumhuriyet University (CUNAM) (Tr), National Center for International Joint Research of Electronic Materials and Systems, International Joint-Laboratory of Electronic Materials and Systems of Henan Province, Henan Key Laboratory of Laser and Opto-electric Information Technology (Cn), Riken Cluster for Pioneering Research (Jp), Zhengzhou Way Do Electronics Co. Ltd. (Cn), and Institute of Materials and Systems for Sustainability (Jp)*

Techniques:

Materials: *GaN, InGaN, AlGaN*

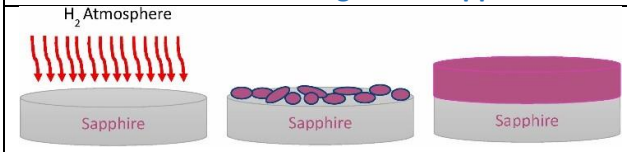
Abstract

InGaN-based quantum wells (QWs) have higher threading dislocation density (TDD) in InGaN Light-emitting diode (LED). Despite of higher TDD, variation of Indium (In) molar fraction in the QW generate localized excitons with higher Indium composition, thus preventing bound carriers from non- radiative recombination. In this work, the sensitivity of the Indium molar fraction in InGaN QWs is explored for near-ultraviolet (UV) LEDs. The theoretically calculated results show that as the Indium composition increases in InGaN QWs, the radiative recombination increases along with an increase in carrier injection efficiency. The reduced non-radiative recombination for higher Indium composition leads to the enhanced spontaneous emission rate and internal quantum efficiency (IQE). For lowered Indium composition, the peak emission wavelength of the InGaN LEDs shift toward the shorter wavelength and the performances degrade drastically. Hence for shorter UV LEDs, the AlGaN-based device structure should be a suitable choice.

OPERA Work Group

WG2

In-situ thermal cleaning of the sapphire substrate and temperature effect on epitaxial AlN



Reference: *Vacuum, 205, 111455 (2022) DOI: 10.1016/j.vacuum.2022.111455*

Authors: *Koçak MN, Yolcu G, Horoz S, Altuntaş İ, and Demir İ.**

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

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

Materials: *AlN/sapphire*

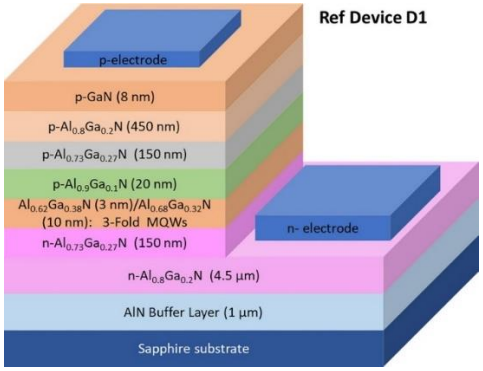
Abstract

The impact of thermal surface cleaning on epitaxial AlN thin films grown on sapphire is investigated in this study at various temperatures. The sapphire substrate is cleaned in a hydrogen environment. Structural, optical, and surface morphology properties of the samples are investigated by using high-resolution X-ray diffraction, Raman spectroscopy, UV–visible spectroscopy, and atomic force microscopy, respectively. Because wastes from the surface of sapphire, which begins to decompose after 1200 °C, cannot be entirely removed at such a low temperature, grain distribution and grain size in the nucleation layer are impacted. Moreover, when a sapphire is cleaned at a high temperature, the rate of breakdown of oxygen atoms from the surface rises, and islands appear on the surface. Roughnesses on the sapphire surface cause misoriented grains and deteriorated the structure. The surface of the sapphire, which is cleaned at 1245 °C, was both sufficiently cleaned and not etched too much, uniformly distributed, and large-sized particles formed in the nucleation layer. Thus, the AlN thin film has grown with high quality in terms of structure, optics, and surface. Experimental results have demonstrated that the in-situ thermal cleaning temperature has a critical influence on the properties of the AlN.

OPERA Work Group

WG2

Performance enhancement of AlGaN deep-ultraviolet laser diode using compositional Al-grading of Si-doped layers



Reference: *Optics & Laser Technology 152 (2022): 108156; DOI: 10.1016/j.optlastec.2022.108156*

Authors: *Sharif MN, Khan MA, Wali Q, Demir I, Wang F, and Liu Y.*

Laboratories: *The Nanophotonics Research and Application Center at Sivas Cumhuriyet University (CUNAM) (Tr), National Center for International Joint Research of Electronic Materials and Systems, International Joint-Laboratory of Electronic Materials and Systems of Henan Province, Henan Key Laboratory of Laser and Opto-electric Information Technology (Cn), Riken Cluster for Pioneering Research (Jp), Zhengzhou Way Do Electronics Co. Ltd. (Cn), and Institute of Materials and Systems for Sustainability (Jp)*

Techniques: *Photonic Integrated Circuit Simulator (PICS3D)*

Materials: *AlGaN, GaN, AlN*

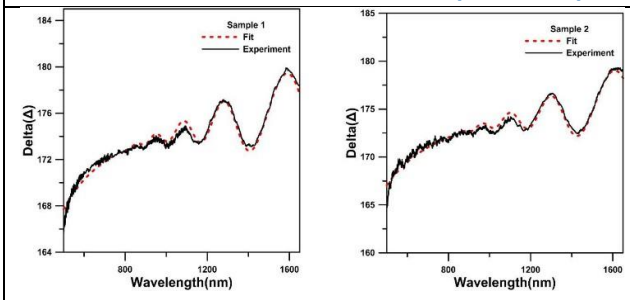
Abstract

Achieving high threshold current density and high optical confinement are big challenges in the realization of high-performance aluminum gallium nitride (AlGaN)-based deep-ultraviolet (DUV) laser diode (LD). In this work, compositional Al-grading of AlGaN layers is used to increase the optical confinement factor (OCF), carrier injection efficiency, gain, and emission power of the DUV LD. Compositional grading of waveguides (WGs) layer, electron blocking layer (EBL), and cladding layers (CLs) demonstrated that the device characteristic can be improved. By using compositional Al-grading of AlGaN p-WG, EBL, p-CL along with n-WG and n-CL, 17.4% OCF, 94.4 mW emission power, and 1369 m^{-1} gain at 267 nm peak emission wavelength are achieved. These improvements are attributed to the reduced threshold current density as well as using better optical confinement scheme in the DUV LD.

OPERA Work Group

WG2

Determination of Optical Properties of MOVPE-Grown InxGa1-xAs/InP Epitaxial Structures by Spectroscopic Ellipsometry



Reference: *Brazilian Journal of Physics 52: 184 (2022); DOI: 10.1007/s13538-022-01187-4*

Authors: *Kaynar E, Sayrac M, Altuntas I, and Demir I*

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

Techniques: *MOVPE, XRD, Spectroscopic Ellipsometry, UV–VIS–NIR Spectrophotometer*

Materials: *InGaAs/InP*

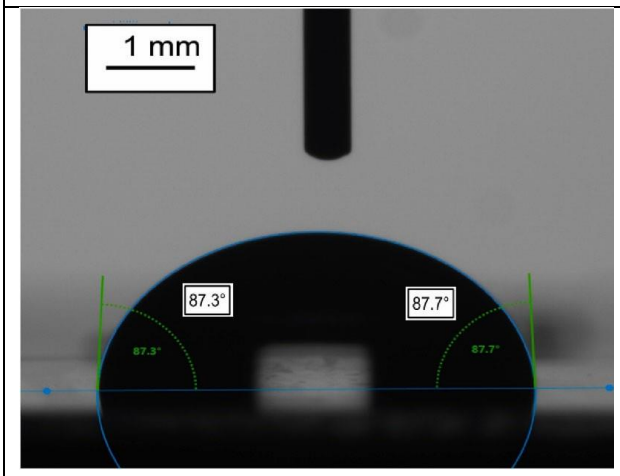
Abstract

$In_xGa_{1-x}As$ epitaxial layers with different AsH_3 flows have been grown on InP substrate with the MOVPE system. It has been found that AsH3 flow variation affects the In concentration of InGaAs/InP structure because the increment of AsH_3 flow increases the In concentration due to the weak bond between In and As. The variation of AsH_3 flow during the growth process has affected crystal quality and optical properties of InGaAs epilayer. The optical properties of the structure have been determined by spectroscopic ellipsometry and spectrophotometer. The variation of In concentration has changed the refractive index value of the structure. The thickness of the samples and refractive index values have been obtained by spectroscopic ellipsometry. The obtained findings show that the reflection has been improved with high AsH_3 flow resulting from surface quality improvement. In addition, it has been observed that the energy band gap has been decreased as a function of the increment of AsH_3 flow because the structure band gap approaches the InAs structure at the high In concentration.

OPERA Work Group

WG2

Optical and nano-mechanical characterization of c-axis oriented AlN film



Reference: *Optical Materials, 129, 112480 (2022); DOI: 10.1016/j.optmat.2022.112480*

Authors: *Panda P, Rajagopalan R, Tripursundari S, Altuntas I, and Demir I.*

Laboratories: *The Nanophotonics Research and Application Center at Sivas Cumhuriyet University (CUNAM) (Tr), and Surface and Nanoscience Division, Materials Science Group, Indira Gandhi Centre for Atomic Research (In)*

Techniques: *MOVPE, XRD, Spectroscopic Ellipsometry, Ultra Nano-indentation Tester, Goniometer*

Materials: *AlN*

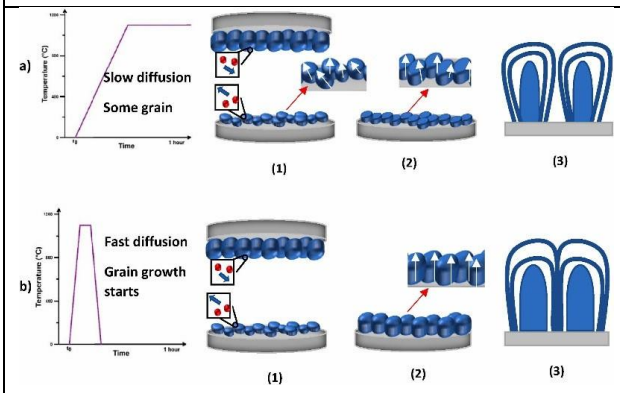
Abstract

This paper reports the temperature effects on the optical properties of metalorganic vapour-phase epitaxy (MOCVD) grown c-axis oriented AlN epilayer thin film studied by in-situ high-temperature spectroscopic ellipsometry. The crystal structure and the quality of the grown AlN epilayer film are analyzed using X-ray Diffraction and rocking curve techniques, respectively. Modelling of the ellipsometric data revealed that the uniaxial anisotropic refractive indices of the c-axis oriented film in the directions $n_{//}$ and $n_{\perp}$ increased from 2.50 to 2.59 and 2.32 to 2.37, respectively with the increase in temperature from 223 to 573 K. The thermo-optic coefficients were evaluated to be around 10^{-5}. Nano-mechanical characterization of this film showed an average hardness of 19.4 GPa at ambient temperature, which is higher than a-axis oriented AlN film. The average surface free energy of the synthesized film as evaluated from contact angle measurements is reported to be around 36.22 ± 0.64 mN/m. These results are highly relevant for a better understanding of c-axis oriented AlN-based materials in high-temperature ultraviolet optical devices

OPERA Work Group

WG2

In-situ and ex-situ face-to-face annealing of epitaxial AlN



Reference: *Vacuum 203 (2022): 111284; DOI: 10.1007/s13538-022-01187-4*

Authors: *Koçak MN, Pürlü KM, Perkitel İ, Altuntaş İ, and Demir İ.**

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

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

Material: *AlN*

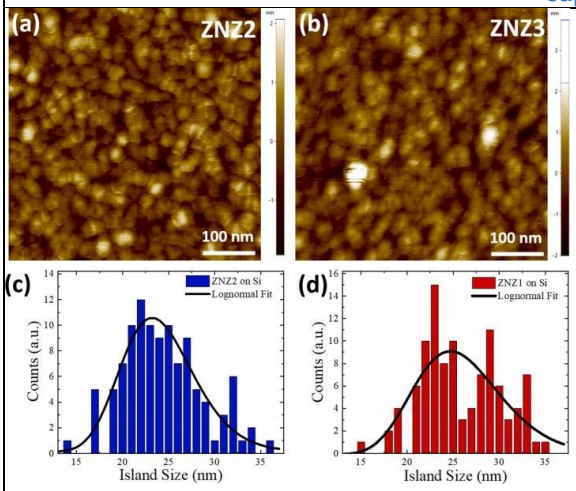
Abstract

AlN films have been deposited on c-plane sapphire substrates by metalorganic-vapor-phase-epitaxy (MOVPE). The changes in the film structure have been investigated by applying different annealing processes which are ex-situ rapid thermal annealing (RTA) and in- situ process after the nucleation-layer (NL). The AlN nucleation-layer grown on sapphire has been annealed face-to-face with ex-situ (RTA) process for 3 min and with in-situ process for 3 h, then pulsed-atomic-layer- epitaxy AlN film has been grown at a high temperature. The samples have been characterized by high-resolution X-ray diffraction, atomic force microscopy, Ultraviolet–visible spectrometry, and Raman scattering to examine the structural properties, surface morphology, and optical properties. The sample annealed with the ex-situ (RTA) process, where rapid diffusion took place, has reached larger grain sizes and the dislocation density has decreased as the grain boundary decreased. Although better crystal quality has been obtained with the ex-situ (RTA) process, it has been observed that the surface roughness of the sample annealed with the ex-situ (RTA) process is higher than that of the sample annealed with the in-situ process. Considering the results, a schematic prediction of the growth process after face-to-face annealing has been proposed. Experimental findings have shown that different annealing processes after growing the AlN-NL have a great effect on the properties of the AlN.

OPERA Work Group

WG2

Magnetic and optical properties of ZnO/Ni/ZnO multilayer film on Si (100) and sapphire substrates



Reference: *Optik, 266, 169595 (2022); DOI: 10.1016/j.ijleo.2022.169595*

Authors: *Kaya D, Akyol M, Tüzemen EŞ, and Ekicibil A.*

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

Techniques: *Radio frequency (RF) magnetron sputtering, XRD, AFM, SEM, UV–VIS–NIR Spectrophotometer, Energy Dispersive x-ray spectroscopy (EDS), and Physical Property Measurement System (PPMS)*

Materials: *ZnO/Ni(t)/ZnO*

Abstract

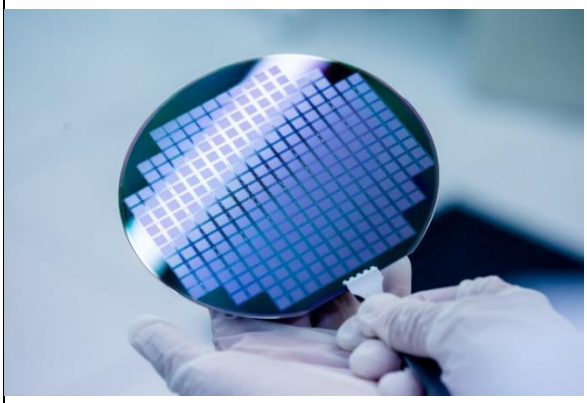
The optical absorption, band gap, and magnetic properties of ZnO/Ni(t)/ZnO multilayer film structures were investigated in various Ni layer thicknesses and substrates. We deposited 1, 4, and 5 nm of Ni film by thermal evaporation technique that sandwiched between ZnO films (~15 nm) via radio frequency magnetron sputtering method on both Si (100) and sapphire substrates. Although x-ray diffraction (XRD) analysis confirmed the (002) crystalline plane of ZnO without any Ni crystal phases on Si (100) surface, the better crystalline directions of ZnO, hexagonal wurtzite structure, was observed on the sapphire substrate. In the XRD analysis, we observed the cubic structure of NiO film formation due to thermally oxidation of Ni ions with interactions ZnO layer. Atomic force microscopy images confirmed the effect of the Ni layer on the average island size of 23.9 ± 2.9 nm and 25.6 ± 6.2 of ZnO films on 4 and 5 nm Ni films, respectively. Energy dispersive x-ray spectroscopy data confirmed that there is no other atom or impurity in the sample structure. The optical transparency of the multilayer films was reduced with increasing Ni layer thickness and maximum transparency was obtained as 97% at 800 nm of wavelength for the film with 1 nm Ni. The direct optical band gap of ZnO/Ni(t)/ZnO films was found to be 3.25, 3.20, and 3.12 eV with the contribution of 1, 4, and 5 nm Ni film in the multilayer film stack. The maximum H_c is found to be 1000 Oe for Si substrates and this value is reduced to around 400 Oe due to the crystal formation of the NiO layer for sapphire substrate samples.

OPERA Work Group

WG2

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

Magnetoresistive thin films and sensors microfabricated in 200mm diameter wafers for microelectronics industry



Reference: *"Spintronic Sensors", Proceedings of the IEEE, 104 (10), pp. 1894 - 1918 (2016); 10.1109/JPROC.2016.2578303*

Authors: *R.Macedo, P. P. Freitas and S. Cardoso*

Laboratories: *INESC MN* ***(Pt)***

Techniques: *Magnetron sputtering, ion beam deposition, magnetic annealing, micro and nanofabrication, laser and UV lithography*

Materials *AMR, GMR and TMR technologies, Epitaxial MgO/CoFeB thin films, thin films with tuneable anisotropies and Resistance, for customized sensor linear ranges.*

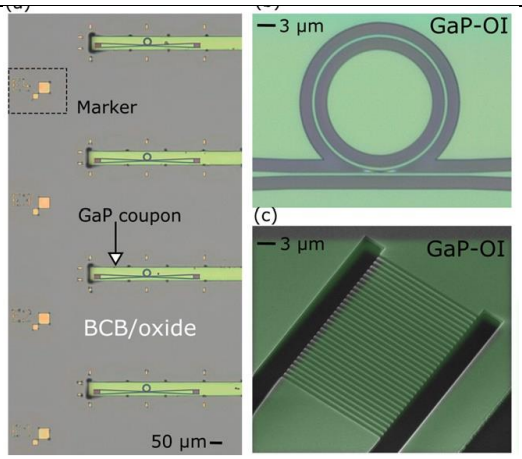
Abstract

Magnetic field sensors, namely, magnetoresistive (MR) sensors have presently a mature level of implementation in the market. The state-of-the-art spintronic sensors used in microelectronics include thin films based on Co, Fe, Ni alloys, prepared typically with 0.2-4.0 nm thicknesses. The different families of magnetoresistance sensors (Anisotropic AMR, Giant GMR and Tunnel TMR) comprise sofisticated multilayer structures, with more than 12 layers, whose thicknesses and interface quality need to be controlled at wafer level, as these impact the final magnetic and electrical performance. For example, integrating an antiferromagnetic film (MnIr, MnPt, MnNi) for exchange coupling with the adjacent ferromagnetic layer is strongly dependent on the grain size control, and interface mixing upon annealing. Another feature for TMR sensors is the precise tuning of the resistance, mediated by the MgO oxide film thickness (usually, 0.8-2nm thick) and its crystallization upon annealing at 360ºC. The keys of success for an industrial qualification are the impressive progress in thin film deposition and characterization tools, which have presently a precision below 0.2nm thicknesses over large area wafers. We have an accumulated know-how on thin film materials growth, sensor design and microfabrication for AMR, GMR and TMR structures, with superior quality in wafers up to 200mm diameter. These are optimized for optimum thermal stability, crossed field resilience, electrical discharge immunity, uniformity, field sensitivity range, noise level and voltage output. The sensors are provided as a service for industrial partners, to cope with the demand of the microelectronics industry, and the growing request for sensors to install in networks of sensors (e.g., for the Internet of Things, and Industry 4.0)

OPERA Work Group

WG3

Gallium phosphide-on-insulator integrated photonic structures fabricated using micro-transfer printing



Reference: *Opt. Mater. Express 12, 3731-3737 (2022); DOI: 10.1364/OME.461146*

Authors: *M. Billet, L. Reis, Y. Léger, C. Cornet, F. Raineri, I. Sagnes, K. Pantzas, G. Beaudoin, G. Roelkens, F. Leo, and B. Kuyken.*

Laboratories: *IMEC-Ghent **(Be)**, NB-photonics **(Be)**, Univ. libre Bruxelles **(Be)**, Institut FOTON **(Fr)**, C2N **(Fr)**.*

Techniques: *MOVPE, ICP-RIE, micro-transfer printing.*

Materials: *AlGaP/GaP*

Abstract

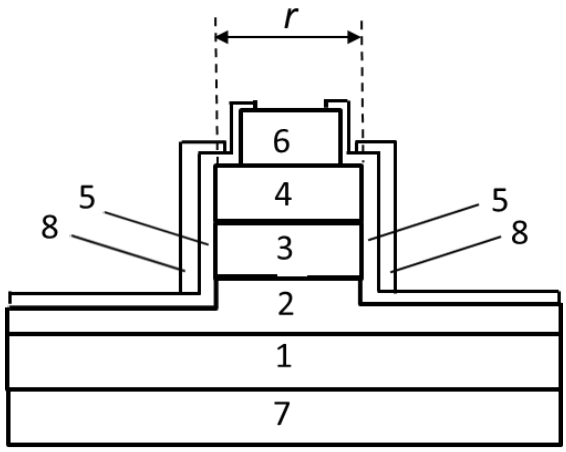
Gallium phosphide-on-insulator emerged recently as a promising platform for integrated nonlinear photonics due to its intrinsic material properties. However, current integration solutions, using direct die-to-wafer bonding, do not support spatially localized integration with CMOS circuits which induce a large and expensive footprint material need.

Here we demonstrate the transfer of gallium phosphide layers to an oxidized silicon wafer using micro-transfer printing as a new approach for versatile future (hybrid) integration. Using this novel approach, we demonstrate as a proof of concept the fabrication of gallium phosphide-on-insulator ring resonators with Q-factors as high as 35,000.

OPERA Work Group

WG2 & WG3

Vertical GaN transistor with insulating channel and the method of forming the same.



Reference: *EPO publication no. EP3714489A1; https://worldwide.espacenet.com/patent/search/family/064949366/publication/EP3714489A1?q=EP3714489*

Authors: *J. Kuzmik*

Laboratories: *Inst. El. Eng., Slovak Academy of Sci. **(Sk)***

Techniques: *MOVPE, RIE*

Materials: *GaN*

Abstract

Invention describes vertical GaN transistor with the insulating channel comprising from the bottom at least:

a conductive GaN substrate (1); a drift n GaN layer (2) formed on the conductive GaN substrate (1); a channel insulating GaN layer (3) formed on the drift n GaN layer (2), wherein residual donors are compensated by impurities and defects; a contacting n^+ GaN layer (4) formed on the channel insulating GaN layer (3); while an electrode (6) of the source is located on the top of the contacting n^+ GaN layer (4), the electrode (7) of the drain is located at the backside of the GaN substrate (1), and the electrode (8) of the gate is located vertically along the channel insulating GaN layer (3) and is separated along its whole length from the contacting n^+ GaN layer (4), the channel insulating layer (3) and the drift n GaN layer (2) by an dielectric insulating layer (5) with a wider energy gap than GaN.

Residual donors in the channel insulating GaN layer (3) are compensated by impurities of carbon, or impurities of iron, or impurities of magnesium or by gallium vacancies.

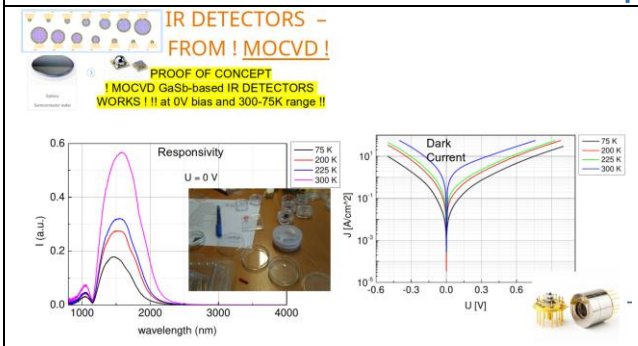
Residual donors in the channel insulating GaN layer (3) are compensated in a way that the concentration of free electrons in the channel insulating GaN layer is less or equal than 10^{11} cm^{-3}.

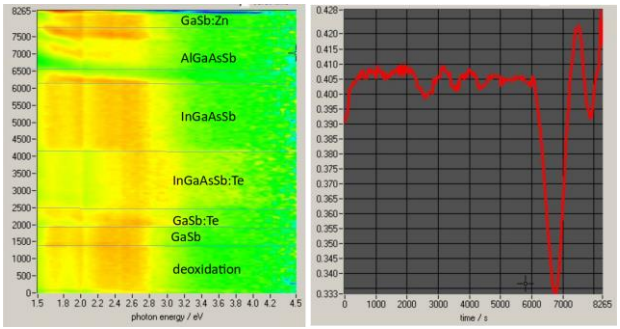
Solution deals also with the method of forming the vertical GaN transistor on the conductive GaN substrate.

OPERA Work Group

WG2 & WG3

MOCVD Growth of antimonide compounds: GaSb, InGaAsSb and AlGaAsSb





Reference: *IC MOVPE XX Conference, Stuttgart 2022,* https://doi.org/10.5281/zenodo.7452380

Authors: *K. Kłos, A. Hospodkova, J. Pangrac*

Laboratories: *Photin (www.photin.eu, **PI**), MOVPE Lab. FZU **(Cz)***

Techniques: *MOCVD, SIMS, I-V, in-situ monitoring RAS.*

Materials: *GaSb-based antimonide semiconductors, InGaAsSb, AlGaAsSb, eSWIR detectors, extended InGaAs*

Abstract

Antimony semiconductors are materials of future for infrared devices: emitters (diode lasers, ICL, QCL) and their integration on Si, eSWIR detectors, TPV cells, MWIR-LWIR detectors (T2SLs), but also new RAM memories (UltraRAM), and TFET transistors. So far most of research on epitaxy of antimonides is carried out in MBE technology, but Photin work on technology of antimonides grown by MOCVD to show it is viable alternative.

This work will share information about growth of GaSb, lattice matched InGaAsSb and AlGaAsSb on (100) GaSb substrates in Aixtron MOCVD equipment, assisted by reflectance anisotropy spectroscopy (RAS) measurement.

The GaSb based structures were grown in an AIXTRON Aix-200 system horizontal quartz reactor with RF heater, non-rotating graphite susceptor and equipped with Laytec EPIRAS 200TT RAS and TrueTemperature measurement. The precursors we used were trimethylindium TMIn, triethylgallium TEGa, tris-tertiarybutylaluminium TtBAl, tertiarybutylarsine TBAs and triethylantimony TESb. Hydrogen was used as the carrier gas with the total flow through the reactor of 10 slpm during deoxidation as well as for the growth of all layers. The total pressure in the reactor was decreased to 150 hPa.

Prior to the epitaxy, the oxide layer from substrates has to be removed. GaSb substrates were etched for 10 min in 35% HCl, then twice rinsed by isopropylalcohol, blowed off by N 2 and directly loaded to the reactor.

The deoxidation of GaSb substrates was carried out under hydrogen atmosphere with 1.5 µmol/min TESb flow at 560 °C for 10 min according to [4]. The growth temperature of GaSb layers was 540 and 560 °C, the later one was used for quaternaries, V/III ratio was kept between 1.8 and 2.5.

The growth processes were in-situ monitored by RAS, which was found as very outstanding method for in-situ monitoring of the quality of epitaxial process of cubic semiconductors.

OPERA Work Group

WG2, WG3