


Summer school on Epitaxy


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Topics

Theoretical concepts
Experimental description
Characterization
Properties of nanostructure
Technological application



Location

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1. A. Anil et al, Ferroic thin films by pulsed laser deposition for the control of thermal conductivity.....p.3
2. A. Besana et al, Low temperature deposition of germanium for SWIR monolithic photodetector integration.....p.4
3. M. Bounab et al, Molecular beam epitaxy of BaTiO_3 assisted by broadband cavity-enhanced optical flux monitoring.....p.5
4. S. Gaddour et al, MOCVD Growth and Characterization of $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ Buffer Layers on Non-Polar a-plane and m-plane Wurtzite CdS substrates for the Epitaxy of Hexagonal $\text{Si}_x\text{Ge}_{1-x}$ Layers.....p.6
5. P. Gadras, Automated growth of DBR supervised by in-situ spectral reflectance measurement.....p.7
6. C. Gutiérrez-Cuesta, Growth mechanism of barium tungstate on $\text{W}(110)$p.8
7. N. Gutmann, Towards bipolar doping of tin monoxide.....p.9
8. J. Kurek, From O-band to LWIR: Growth Optimization of Quantum Structures via Metal-Organic Chemical Vapour Deposition (MOCVD).....p.10
9. C. Lourdiane, Development and study of a laser compatible with the industrial Si platform.....p.11
10. A. Muriel, Multi-scale study of metallic thin films growth: impact of process parameters on early growth stages.....p.13
11. J. Ngufo, Development of WTe_2 /Sapphire for spin-orbitronics applications.p.14
12. A. Oliveira, Ge-on-Si dual-band detectors for solvents recognition.....p.15
13. A. Sauvagnat, SAG-HVPE of InGaN NWs for the realization of InGaN micro-substrates: a promising way to efficient nitride-based red emission.....p. 16
14. N. Stegamat, Epitaxial Growth and Characterization of 2-Dimensional GaSe/InSe for High-Frequency and Optoelectronic Applications.....p.17
15. Toschi, $V_{\text{N}}\text{-}V_{\text{In}}$ divacancies as the origin of non-radiative recombination centers in InGaN quantum wells.....p.18
16. K. Wang, Kinetic Monte Carlo Simulation of Epitaxial Growth of 2D Si.....p 19
17. A. Yadav, *In situ* GIXRD study of epitaxial CuO films grown on $\text{SrTiO}_3(001)$ and LaAlO_3 by oxygen-plasma-assisted MBE.....p.20

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Ferroic thin films by pulsed laser deposition for the control of thermal conductivity

The development of thermal conductivity switches to control heat flows [1] would significantly improve the efficiency of thermoelectric devices and solid-state refrigeration systems and pave the way for computing with heat [2]. Seminal works demonstrate that ferroics, e.g. ferroelastics and (anti)-ferroelectrics are suitable materials to design thermal conductivity switches [3,4,5]. Their ability to tune thermal conductivity depends on two main mechanisms: domain structures, including domain walls, and phase transitions. Here we explore how ferroelectric and antiferroelectric thin films grown by pulsed laser deposition could be used to design a compact and efficient thermal conductivity switch operating over a wide temperature range.

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Low temperature deposition of germanium for SWIR monolithic photodetector integration

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

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

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

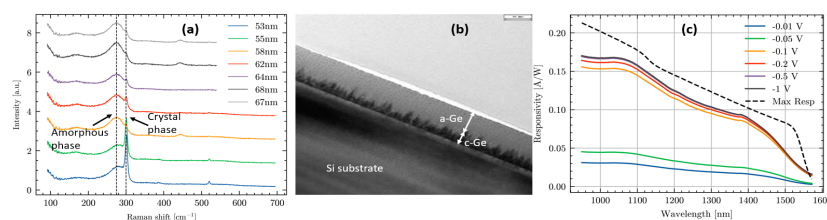


Figure 1: (a) Raman spectra of Ge crystalline-amorphous phase transition at 200°C. (b) TEM image of crystalline and amorphous interface in Ge epilayer at 200°C. (c) Measured responsivity at different bias and comparison with the maximal achievable responsivity.

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Molecular beam epitaxy of BaTiO₃ assisted by broadband cavity-enhanced optical flux monitoring.

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Barium titanate (BTO) thin films attract attention because of their remarkable ferroelectric properties and large optical non-linearities. They can be used in a wide range of applications, such as ceramic capacitors, non-volatile memories, piezoelectric sensors and actuators, and electro-optic modulators [1]. Molecular beam epitaxy (MBE) allows the growth of very high-quality BTO on oxide substrates, as well as on Si, Ge, and GaAs using SrTiO₃ templates [2].

MBE growth of BTO must be carried out under high oxygen plasma pressure (typically about 10⁻⁵ Torr) to ensure sufficient oxidation of the material and good ferroelectric properties. [3]. This is highly challenging, as these oxidizing conditions induce Ba and Ti flux drift, causing composition imbalance in the BTO thin layer.

In this contribution we will show how a home-made high sensitivity atomic absorption setup (broadband cavity-enhanced optical flux monitoring, BBCE-OFM [4]) can be used in-situ to control MBE BTO growth under oxidizing conditions by enabling real-time compensation for Ba and Ti flux drift. BBCE-OFM is chemically selective and independent on the operating chamber oxygen pressure. BTO grown using this strategy exhibits high epitaxial quality, as confirmed by RHEED and XRD measurements.

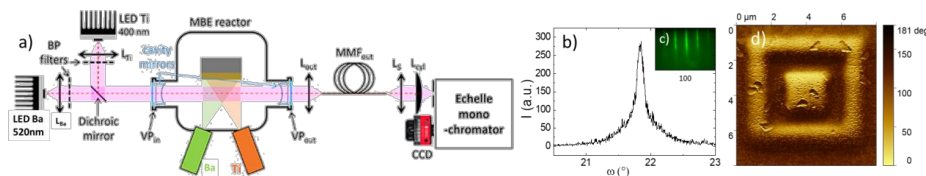


Figure 1: a) BBCE-OFM schematic, b) Rocking curve measured on the 002-peak c) RHEED patterns after growth d) phase image of piezoresponse force microscopy

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Automated growth of DBR supervised by in-situ spectral reflectance measurement

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In-situ measurement is a key feature to better understand and precisely control the growth of complex structures, such as VCSEL [1–3]. In this work, we are showing the automated growth of a GaAs/AlAs Distributed Bragg Reflector (DBR) centred at 940 nm, feedback controlled with in-situ spectral reflectance measurement and realized without preliminary accurate cell flux calibrations. This method relies on the measurements of the refractive indices' dispersion over wide spectral range (400 – 1400 nm) at growth temperature (600°C) of $Al_xGa_{1-x}As$ alloys, which are shown in **Erreur ! Source du renvoi introuvable.-a**). To do so, in-situ reflectance measurement is used combined with ex-situ layer thickness and composition measurement by X-ray diffraction. Afterwards, the spectral reflectance of the targeted GaAs/AlAs DBR is calculated using the refractive indices dispersion previously determined. The DBR is grown by switching from one layer to the next one when we measure in-situ a signal extremum at the optimal wavelength [3] for this layer, without any need for cell calibration. After the growth, this sample is characterized by X-ray diffraction and Fourier transform infrared reflectance, as shown in Fig. 1-b), resulting in a very good agreement compared to the targeted stop-band central-wavelength.

This work was partially supported by LAAS-CNRS and the the French Renatech network, and founded by EPICENTRE, a joint laboratory between RIBER and LAAS-CNRS

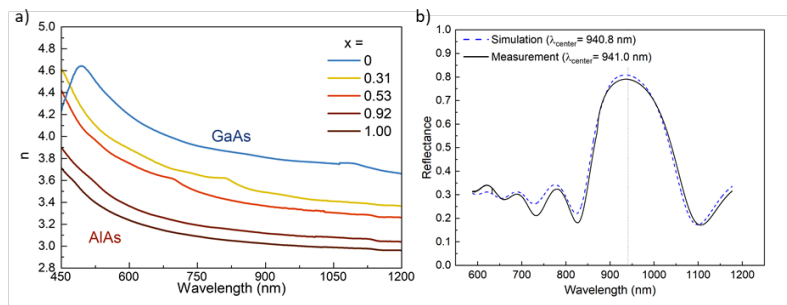


Fig. 1: a) Measured refractive indices of $Al_xGa_{1-x}As$ at 600°C, b) Simulated reflectance spectrum (blue) and FTIR measurement of our Automatic DBR (black). The central wavelength of the stop band of the simulation and the measurement are merged (dotted vertical line).

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MOCVD Growth and Characterization of $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ Buffer Layers on Non-Polar a-plane and m-plane Wurtzite CdS substrates for the Epitaxy of Hexagonal $\text{Si}_x\text{Ge}_{1-x}$ Layers

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Research on III-V, II-VI, and IV-IV semiconductors has been highly active, leading to new insights in fundamental physics and offering exciting opportunities for electronics and photonics. One effective strategy for modifying the properties of these materials is by studying their different crystal forms, known as polytypes. This structural variation can significantly alter semiconductor properties, such as converting an indirect bandgap to a direct bandgap, thereby enhancing light-emission efficiency for optoelectronic applications. Additionally, switching between crystal phases (such as from cubic to hexagonal) can improve material stability, reduce defects, and increase carrier mobility, factors that are essential for optimizing device performance.

Similar strategies are now applied to group IV semiconductors, particularly $\text{Si}_x\text{Ge}_{1-x}$. Its hexagonal structure exhibits a direct band gap (contrary to indirect cubic SiGe) and excellent light-emission properties, with a tunable mid-infrared emission wavelength ranging from 1.8 to 4.2 μm for silicon concentrations between 0% and 40%. The main objective of this study is to grow hexagonal $\text{Si}_x\text{Ge}_{1-x}$ layers on bulk wurtzite substrates with a-plane and m-plane orientations ($\{1-100\}$ and $\{11-20\}$, respectively). Since bulk GaAs does not exist in the wurtzite phase, alternative CdS substrates were selected as hexagonal templates. These substrates exhibit non-polar surface orientations and have lattice parameters compatible with those of Si and Ge.

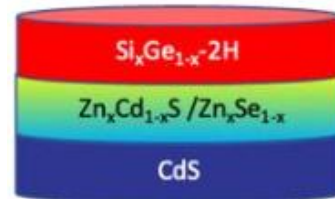


Figure 1 : Growth of $\text{Si}_x\text{Ge}_{1-x}$ -2H layers

Despite the promising properties of hexagonal Ge, the synthesis of high-quality Ge-2H layers remains challenging. Current methods are mostly limited to nanostructures, which restrict active volumes and hinder the scalability of device fabrication. To overcome this limitation, we propose the introduction of a wurtzite $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ buffer layer, enabling better integration of this material into advanced optoelectronic devices and improving the epitaxial growth of WZ-SiGe layers.

In this study, $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ epilayers were deposited on commercially available single-crystal CdS substrates with a-plane and m-plane orientations using the MOCVD technique. This low-temperature process enables large-area epitaxial growth with high chemical purity. However, one key challenge lies in substrate surface preparation, as CdS surfaces are prone to oxidation and the resulting oxide layer is difficult to remove. We investigate the effect of both chemical and thermal surface treatments on the interface quality prior to growth. The MOCVD-grown layers were characterized by X-Ray Diffraction (XRD) and Scanning Electron Microscopy (SEM).

Growth mechanism of barium tungstate on W(110)

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In this work we will explore the W–O interaction at the W(110) surface and its central role in the growth mechanism of these complex oxide nanostructures. Tungsten has been a key substrate in surface science since its birth, due to its high thermal stability, low solubility, and high melting point. However, very little is known regarding its use when growing oxides. We have observed how, surprisingly, the process leads to the formation of tungstate nanostructures while growing a metal on W(110) by high-temperature molecular beam epitaxy in an oxygen atmosphere. We present the growth of BaWO₄ islands by high-temperature oxygen-assisted molecular beam epitaxy (MBE) on a W(110) substrate. The surface evolution was monitored in real time by Low-Energy Electron-Microscopy (LEEM)[1]. We studied the structural properties of the islands in real space by LEEM and in reciprocal space by Low Energy Electron Diffraction (LEED). We obtained the chemical composition of the structures by x-ray photoemission spectroscopy and x-ray absorption in Photoemission Microscopy (PEEM). Furthermore, we imaged the islands by Thermionic Emission Microscopy when the sample was heated above 700 C and studied the emission dependence of the nanostructures termination. We propose that tungstate formation is driven by the surface mobility of W⁶⁺ species generated during the reaction with oxygen.

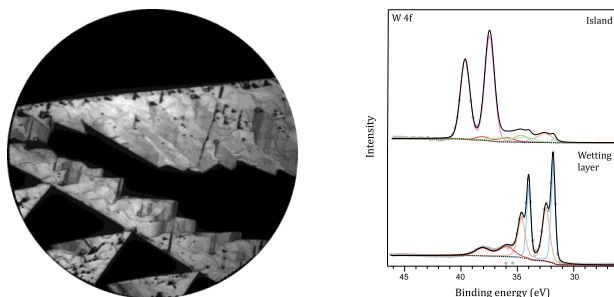


Fig 1. Left, ThEEM image of BaWO₄ island, FOV 10μm. Right, XPS spectra on islands and wetting layer.

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Towards bipolar doping of tin monoxide

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Transparent conducting oxides (TCOs) are essential components in optoelectronic devices; however, achieving stable *p*-type conductivity remains a significant challenge for most oxide materials. Tin monoxide (SnO) stands out as a rare example of an oxide exhibiting native *p*-type conductivity [1], making it a promising candidate for bipolar doping and the realization of oxide-based *pn* homojunctions. Recent studies have demonstrated that the electrical properties of SnO can be tuned from highly *p*-type conductive to semi-insulating through *p*-type doping with Ga and compensating donor doping with La [2]. Additionally, theoretical predictions suggest the potential for *n*-type doping of SnO using elements such as Y, Al, and Sc [3].

In this work, we present experimental investigations of Ga- and Al-doped SnO thin films grown via suboxide molecular beam epitaxy (S-MBE), as illustrated in Fig 1a). An *in-situ* reflection high-energy diffraction (RHEED) image an Al-doped SnO films is shown in Fig. 1b). *Ex-situ* characterization of the films includes Hall and van der Pauw measurements for electrical properties, while surface morphology and crystal quality are assessed using atomic force microscopy (AFM) and X-ray diffraction (XRD), respectively.

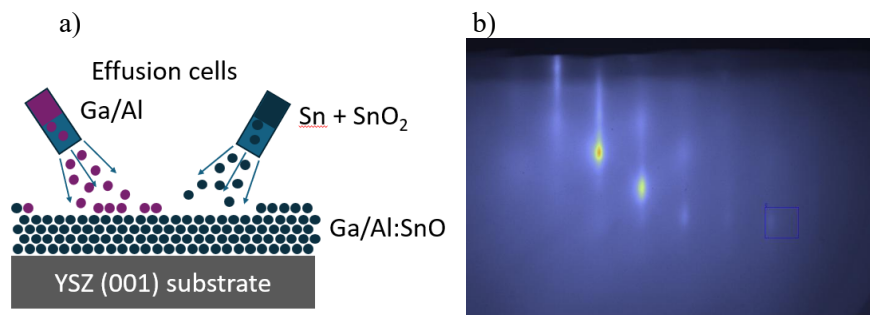


Figure 1: a) Schematic of S-MBE. b) *in situ* RHEED image of an Al-doped SnO thin film.

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From O-band to LWIR: Growth Optimization of Quantum Structures via Metal-Organic Chemical Vapour Deposition (MOCVD)

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This work demonstrates the successful transfer of quantum structures epitaxy from laboratory research to industrial-scale production via Metal-Organic Chemical Vapor Deposition (MOCVD). We employ the AIXTRON 2800 G4™ multi-wafer planetary reactor – capable of processing 12 wafers per run – for the precise and reproducible growth of advanced quantum heterostructures designed for broadband infrared optoelectronic applications.

We report on the development and optimization of InAs/InP quantum dots (QDs) for telecom-band emission, as well as strain-balanced InGaAs/InAlAs quantum cascade laser (QCL) heterostructures operating across the 3.8–13 μm mid- to long-wave infrared (MWIR–LWIR) range.

Transferring these sophisticated epitaxial processes to a high-throughput, production-oriented environment presents several challenges. The complexity and subtleties of growing high-quality quantum structures require precise control over layer parameters throughout the lengthy deposition process.

In the case of self-assembled quantum dots (QDs), droplet crystallization poses specific difficulties, including the arsenic/phosphorus (As/P) atom exchange, which necessitate understanding of the crystallization kinetics and special growth conditions development. Additional challenges involve precise control over the geometry (symmetry), density, and size of the QDs to ensure uniformity and target emission properties. For quantum cascade laser (QCL) structures, the epitaxy involves more than 1000 layers and total thicknesses exceeding 10 μm, placing stringent demands on compositional uniformity, thickness accuracy, and interface sharpness. Special attention was given to achieving abrupt interfaces by optimizing growth interruption times and minimizing the exposure of layers to oxygen contamination in the reactor – striking a balance between interface sharpness and material integrity. Another key challenge was to maintaining a level of precision in layer thickness and composition sufficient to enable fabrication of devices with the desired emission wavelength and optical performance. For process monitoring and structural evaluation, high-resolution X-ray diffraction (HR XRD) and transmission electron microscopy (TEM) were employed. Surface morphology was analysed using differential interference contrast (Nomarski) microscopy, atomic force microscopy (AFM) and scanning electron microscopy (SEM). Doping profiles and impurity levels were assessed via secondary ion mass spectrometry (SIMS).

These results underscore the feasibility of using industrial MOCVD platforms for the reproducible, high-quality growth of advanced quantum nanostructures tailored for infrared optoelectronic applications.

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Development and study of a laser compatible with the industrial Si platform

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Summary of the poster:

The telecommunications sector is constantly evolving to meet the growing demand for bandwidth [1], requiring ever more efficient, cost-effective, and energy-saving photonic components. One way to make these photonic devices is by the integrating III-V semiconductors on silicon [2], enabling us to benefit from both the industrial maturity of the Si platform and the advanced optical properties of the III-V platform. The InP monolithic platform was developed using a thick vertical p-i-n junction as a core structure for active components. This > 2 μm -thick vertical structure allows for lower access resistance [3], efficient carrier injection [4] and reduced optical losses by distancing the metal contact from the active region [5].

III-V integration on Si can be done using different methods: (i) the monolithic approach that consists of the direct growth of III-V layers on a Si wafer, but remains challenging to allow for high quality III-V epitaxial layer stacks, due to their different material properties (large lattice mismatch, different thermal expansion coefficients and surface polarity) [6], (ii) the heterogeneous approach by bonding the III-V layer previously grown on III-V to a Si wafer, while allowing to overcome the intrinsic material differences, isn't adapted to InP building blocks that integrate multiple active sections due to their topology making them incompatible with bonding specifications [7]. More recently, a third integration method has emerged to overcome these challenges: (iii) the heterogenous integration by bonding and regrowth [8], allowing us to transpose the full epitaxial toolkit based on several regrowth steps from the monolithic InP platform into the III-V/Si platform. It consists of regrowing III-V materials on a thin layer of InP that has been bonded to a SOI wafer.

Regardless of the integration method, fully transferring the know-how of the monolithic InP platform by III-V/Si integration requires adaptations of the Si platform to InP-specific constraints associated with the use of vertical p-i-n junction to allow lossless III-V/Si optical coupling from the III-V waveguide to the Si waveguide. When trying to optically couple these two waveguides, the difference in the effective indexes between the two results in significant optical losses. Several solutions were proposed, either by adding a-Si layer in certain areas to locally increase the thickness [9], by using an SiGe alloy to enhance the Si's waveguide refractive index [10], or by using a lateral p-i-n junction to reduce the III-V guide's thickness locally [11].

Yet, the ultimate goal is to transfer all these know-hows on the existing industrial Si platform used by foundries, that was developed using a 220 nm waveguide [12]. This study aims to provide solutions by morphologically and electrically validating a new design proposed by the III-V Lab presented in Figure 1a. Based on optical simulations shown in Figure 1b, the latter allows for a lossless optical transition (97% transmission) between a vertical PIN junction that forms the III-V waveguide and the 220 nm-thick Si waveguide, based on what we call a "remote head" P contact. From a practical standpoint, this design can be achieved from a first regrowth step of InP:SI followed by a second InP:P regrowth which is etched right above the active zone. By locally decreasing the III-V waveguide thickness—through lateral offsetting of the InP:P layer—while maintaining a vertical current path (dotted white line in Fig. 1.a), the effective indexes of the two waveguides can be closely matched. This enables an efficient optical transition, as illustrated in Fig. 1.b.

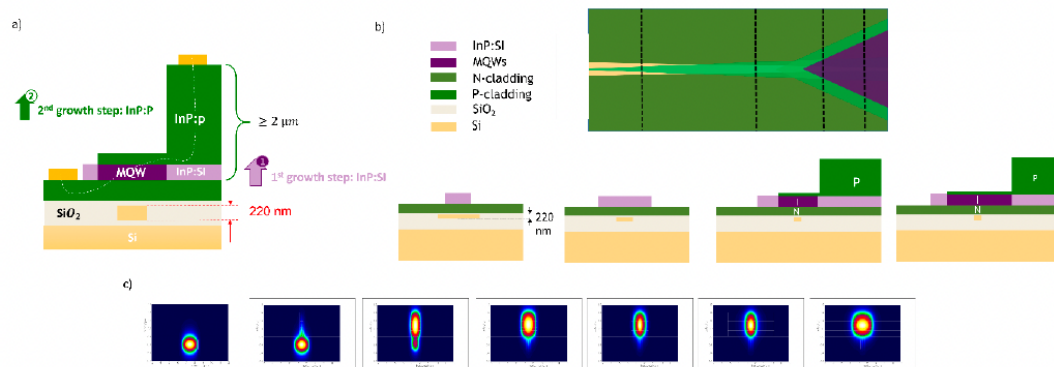


Fig. 1 : (a) Cross-section sketch of the vertical p-i-n junction structure with the "remote head". (b) Description of the III-V/Si transition using the proposed III-V vertical structure. (c) Optical simulations of the III-V/Si transition.

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Title: Multi-scale study of metallic thin films growth: impact of process parameters on early growth stages

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Metallic thin films are essential in modern technologies such as microelectronics and optoelectronics. The microstructure and resulting properties of these films are intricately dependent on deposition conditions, including the kinetic energy of incoming particles, substrate nature and temperature, and the characteristics of the deposited species (e.g., surface mobility, chemical reactivity). Experimental control over these parameters is allowed by magnetron sputtering deposition, commonly employed for thin film growth.^[1] While homoepitaxial metal deposition has been extensively studied,^{[2],[3]} the mechanisms governing heteroepitaxial deposition remain less well understood. Elucidating the initial stages of heteroepitaxial growth is the primary objective of this work aiming at assessing their impact on film microstructure (grain size, texture) and properties.

In this study, we use density functional theory (DFT) to investigate the stability of various atomic configurations during the early stages of copper deposition on silicon (001)–(2x1). We assess the thermodynamic properties of the reconstructed Si surface in contact with incoming Cu atoms, revealing key insights into preferential adsorption sites and single-atom diffusion mechanisms. Furthermore, we evaluate the relative stability of small cluster configurations (2 to 5 atoms) at low surface coverage, providing energy differences that clarify whether island growth or 2D growth is favored. The influence of neighboring islands is also examined using periodic boundary conditions on the surface slab. Ultimately, this work aims to enable more accurate modeling of heteroepitaxial thin film growth at later stages, using methods capable of simulating larger systems over realistic timescales.^[4]

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Development of WTe₂/Sapphire for spin-orbitronics applications

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2D Transition metal dichalcogenides (TMDs) have created huge research interest due to their unique properties and potential for various applications in energy, electronics, photonics, and spintronics. TMDs are mainly obtained through mechanical or chemical exfoliation of bulk crystals into thin atomic layers. Despite challenging, epitaxial growth of these materials offers significant advantages, including the production of high-quality films, possible long range in-plane ordering and precise control over layer thicknesses, making it more suitable for applications [1]. Insulating substrates like sapphire (Al₂O₃) are important for more reasons: electrical insulation, reduced (if any) charge transfer, optical transparency, size, crystalline symmetry (a-plane, c-plane, r-plane and m-plane) [2]. TMDs share MX₂ structure (M=W, Mo and X=Te, Se, S). Among TMDs, WTe₂ is the only one for which the Td phase is the most energetically favored [3]. It has been predicted to be a quantum spin Hall insulator with bandgap opening due to spin-orbit coupling [4]. It has also been demonstrated to be ferroelectric down to 2 ML [5].

In this study, we elaborate the growth of WTe₂/Sapphire (a-plane and c-plane) by molecular beam epitaxy, and the preliminary results show firstly a polycrystalline growth due to either a Te deficit or an excess of W in the composition. High temperature annealing (about 600°C) under Te environment is necessary to improve the growth, which allowed us to obtain more crystalline films. XRD and Raman were performed to characterize the growth. XRD shows a peak at about 12.52° in 2 theta corresponding to the (002) WTe₂ plane family, which is the most intense peak. Raman shows well defined peaks of WTe₂ and this is in good agreement with previous works [6]. We have also elaborated several samples (different thicknesses) of WTe₂/ML-Graphene/SiC by MBE [7] for ARPES and XPS measurements. Angle-resolved photoemission spectroscopy (ARPES) show electron-pockets (for 1-ML and 4-ML) at the Fermi level, in agreement with DFT calculations performed on free-standing Td-WTe₂ and previous reports [8]. This confirms the crystalline quality of the films. Fermi surface measurements evidence three equivalent domains rotated by 120° with respect to each other that correspond to different orientations of the WTe₂ orthorhombic unit cell on ML-graphene. We also observed a bandgap opening due to spin-orbit coupling. XPS exhibit the characteristics peaks of 4d-Te and 4f-W.

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Ge-on-Si dual-band detectors for solvents recognition

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Light sensing beyond the visible spectra has always played an important role in scientific advances. By connecting two photodiodes in a back-to-back architecture, creating a dual-band detector, it is possible to sense in two different spectral regions depending on the semiconductor band gap and applied voltage bias [1]. Those features allow such devices to operate without any mechanical or dispersive elements, acquiring spectral information at pixel level in two different bands, data which could be reliably combined to provide information that neither band can give by itself.

Here, we resort on a Ge-on-Si dual-band detector, capable of sensing from visible and near-infrared (Si photodiode) to short-wave infrared (Ge photodiode) to discriminate between different solvents.

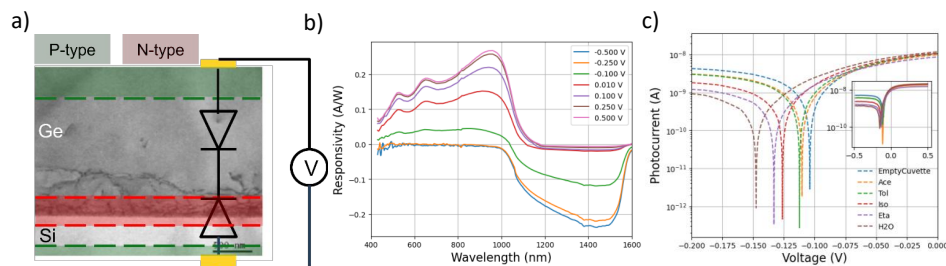


Figure 1- (a) Schematic representation of the dual-band detector (b) Device responsivity measured for several voltage bias (c) photocurrent-voltage curves for the different solvents in measure.

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SAG-HVPE of InGa_{0.5}N NWs for the realization of InGa_{0.5}N micro-substrates: a promising way to efficient nitride-based red emission.

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InGa_{0.5}N material is widely studied for high-performance optoelectronic devices due to its tunable bandgap from infrared to ultraviolet by varying the mole fraction of indium in the alloy. However, growing InGa_{0.5}N layers on commonly used low-cost substrates presents considerable challenges, notably due to compressive stresses, segregation phenomena and indium instability at high growth temperatures, resulting in a reduction of external quantum efficiency (EQE), particularly for red wavelengths. These limitations could be overcome with the nanowire (NW) geometry, which enables InGa_{0.5}N material to be grown with low defect density by propagating stress laterally. Optical quality depends on the substrate, but the use of InGa_{0.5}N NWs as seeds for micro-substrates looks promising. With its high growth rates, hydride vapor phase epitaxy (HVPE) offers a promising method for the controlled and fast growth of InGa_{0.5}N NWs, paving the way for a new generation of optoelectronic devices [1,2,3,4].

In this study, the full range of indium composition is obtained by controlling the input partial pressures of the group III elements (InCl₃ and GaCl) and the growth temperature. Thanks to the use of chlorinated precursors, selective area growth (SAG) of well-ordered InGa_{0.5}N NWs with indium composition ranging from 0 to 100% is achieved. Photoluminescence (PL) measurements are carried out to study the optical properties and compositions of the NWs. Experimental results from systematic studies are supported by a phenomenological model of the top-plane InGa_{0.5}N NW growth. The step-by-step growth mechanism, and the processes of III elements adsorption, diffusion, and chlorine desorption by one mechanism have been considered. InN kinetic modelling is achieved by using the Eyring theory. The fitting of experimental points allows to determine the behavior of the indium composition in the solid phase with increasing temperature at different vapor phase compositions. No indium content gap is observed for the growth of vapor-solid InGa_{0.5}N structures by HVPE. These results are promising for the production of InGa_{0.5}N micro-domains and pave the way for the realization of RGB nitride-based pixels.

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Epitaxial Growth and Characterization of 2-Dimensional GaSe/InSe for High-Frequency and Optoelectronic Applications

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This poster will show some recent results in the growth of 2D materials, specifically Gallium Selenide (GaSe) and Indium Selenide (InSe) on Silicon (111) substrate wafer. These materials fall into the III-VI family and a design of their structure can be seen in figure 1. MX (M = Ga, In and X = S, Se, and Te). The growth is done via Molecular Beam Epitaxy (MBE) and thus is quite relevant to the theme of the MatEPI Summer school. In our case, the growth more closely resembles van-der-waals (VdW) epitaxy which was developed in 1980 by Matthew Koma [2]. This is how we are able to use a Silicon substrate with an in-plane lattice constant that is $>10\%$ different from the deposition material. The ultimate goal for this project is to grow InSe on GaSe on Silicon(111). GaSe here functions just as a buffer layer to avoid any surface related effects and InSe will serve as the channel for a field-effect-transistor. The project began in January 2025 and is not complete, but I plan to show a lot of the characterization data we've gathered on our GaSe films. We also have some preliminary experiments with InSe on Silicon which will be put on the poster as well. Some of the characterization techniques we've used include atomic force microscopy (AFM), x-ray photoelectron spectroscopy (XPS), reflection high-energy electron diffraction (RHEED), out of plane and in-plane grazing incidence x-ray diffraction (XRD), Raman spectroscopy, and

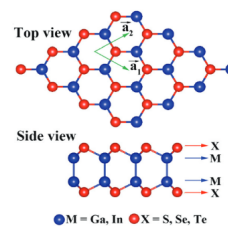


FIGURE 1 – Top and side views of MX Monolayer Crystal Structures [1]

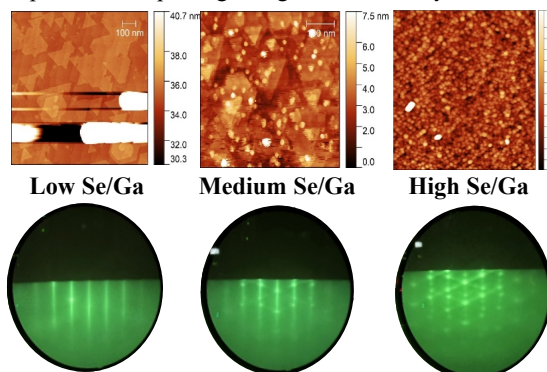


FIGURE 2 – Se Cracker Cell a) AFM Images (1 μm) and b) Rheed Pictures of Se/Ga Ratios

scanning electron microscopy (SEM). Figure 2 shows an example of some of the AFM and in-situ Rheed results obtained. I also plan to present the impact that substrate temperature, cell source, and Group VI : Group III flux ratio all have on the phase, morphology, and quality of the films.

**V_N - V_{In} divacancies as the origin of non-radiative recombination
centers in InGaN quantum wells**

Authors : A. Toschi, Y. Chen, J.-F. Carlin, R. Butté, N. Grandjean

The efficiency of InGaN/GaN quantum wells (QWs) in blue light-emitting diodes is significantly influenced by point defects (PDs) originating in the high-temperature (HT) GaN buffer and forming non-radiative recombination centers (NRCs) in the QW [1]. While an InGaN underlayer (UL) prevents PDs from reaching the QW [2], the nature of these defects, their migration and incorporation into the QW remain poorly understood.

In this study, we explore the nature of PDs generated during the growth of the HT-GaN buffer and their incorporation into InGaN QWs grown using metalorganic vapor phase epitaxy. Our investigation starts on understanding the migration pathways of these PDs from the HT-GaN buffer into the QW, considering two potential mechanisms: diffusion [3] and surface segregation [4]. A diffusion model predicts increased defect concentration in the InGaN QW with growth interruption (GI) before the QW growth, whereas surface segregation phenomenon does not. Photoluminescence measurements on samples with increasing GI durations reveal no degradation in QW efficiency, supporting surface segregation as the dominant migration mechanism. Furthermore, we show that the QW efficiency is not affected when a HT-GaN layer is deposited above the QW, confirming that defect migration occurs exclusively toward the surface.

To gain deeper insight into the nature of these defects, we investigate the stability of the HT-GaN surface under different combinations of temperature and ammonia flow conditions. Our results reveal that higher annealing temperatures or lower ammonia flows promote defect formation, strongly indicating the formation of nitrogen vacancies (V_N), also theoretically predicated to have the lowest formation energy in GaN [5]. However, being V_N shallow defects, they cannot be themselves the NRCs in InGaN QWs degrading their efficiency but they may form more complex defects. We propose that V_N are created at the HT-GaN surface due to its low stability and segregate toward the surface due to their lower formation energy there with respect to the bulk. However, in In-containing layers, where indium vacancies (V_{In}) are abundant due to the weak In-N bond, they interact with V_N to form V_N - V_{In} divacancies, which are incorporated into the layer and act as effective NRCs.

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Kinetic Monte Carlo Simulation of Epitaxial Growth of 2D Si

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The first 2D material, graphene, was discovered in 2004 by exfoliation. It attracted much attention because of its remarkable properties which are different from graphite. However, the limitations of graphene, such as a small band gap, integration challenges, and optical properties, have spurred exploration into alternative 2D materials. Silicene, 2D material of silicon, stands out as a promising candidate. Unlike graphene, silicene lacks a pi-stacking structure, making exfoliation impossible. Epitaxy, known for producing high-quality materials, is thence the only method for silicene synthesis.

The epitaxial growth of 2D Si on Ag(111) [1] and double layer Graphene/SiC substrates [2] reveals unexpected growth modes. On Ag(111), Si atoms can insert into the substrate surface, forming inserted islands at high temperature ($T \geq 300\text{K}$). On the double layer Graphene/SiC, Si forms three distinct types of islands: 3D fractal islands, 2D hexagonal flakes with a surrounding ring, and 2D irregular flakes with a surrounding ring.

To rationalize these anomalous growth modes, we develop an out-of-equilibrium description of a lattice-based epitaxial growth model, which growth dynamics are analyzed via kinetic Monte-Carlo simulations where the process rate depends on the type and number of nearest neighbor atoms. For the Ag(111) case, we introduce intermixing effects between Si and Ag atoms. Through meticulous analysis of atomic microscopy images and island density fitting, we successfully reproduce both qualitatively and quantitatively the anomalous growth patterns of Si on Ag(111) [3].

As regards, growth of silicene on Graphene/SiC, we derive a model that revisits the classical dewetting thermodynamics, incorporating adsorption energies and step-edge effects. The out-of-equilibrium dynamics computed by kinetic Monte Carlo simulations reproduce the flake morphologies, and transformation into non-coalescent dendritic pyramids. The present modeling and understanding of the mechanisms at work in these systems are the first building blocks for future systematic studies aimed at controlling and growing large silicene flake.

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In situ GIXRD study of epitaxial CuO films grown on SrTiO₃(001) and LaAlO₃ by oxygen-plasma-assisted MBE

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CuO tenorite has a monoclinic structure and is paramagnetic at room temperature while other members of 3d transition metal monoxides have cubic rocksalt structure. Thin tetragonal films (t-CuO) can be obtained by epitaxy on SrTiO₃(001) [1]. Its structure is similar to rocksalt one, but shows a tetragonal distortion. The c/a ratio of t-CuO is large, which reduces interplanar coupling giving a 2D character, a feature observed in high-T_c superconductors. This suggests that these films could be made superconductors by doping. The structure of CuO thin films grown on SrTiO₃(001) (STO) and on LaAlO₃(001) (LAO) by OPA-MBE was studied using GIXRD. On both substrates CuO grows tetragonal, with a lattice constant ratio c/a of 1.35 and 1.5 for STO and LAO respectively, and in coherent epitaxy up to a thickness of more than 7 nm (13 U.C.) for STO. Moreover, the Cu-O-Cu bonding angle of 180° strengthen the super-exchange interaction with respect to the monoclinic phase, improving the CuO magnetic properties [2]. Room temperature ferromagnetism is expected for Fe (Co) doped t-CuO films. We aim at growing room temperature magnetic semiconductors by replacing a fraction of Cu with Co. Doped film (t-Co_{0.1}Cu_{0.9}O/STO) were also grown with c/a ratio of 1.34. Investigation of magnetic properties of such films is in progress.

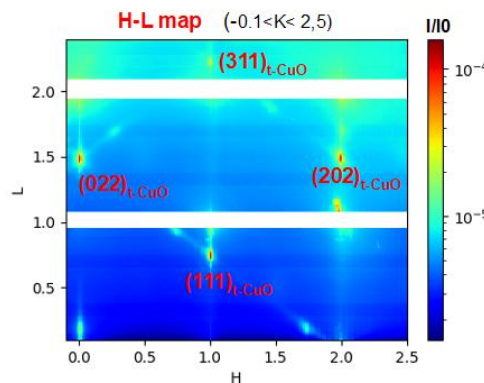


Figure 1: Reciprocal space map of the X-ray diffracted intensity measured on 7nm CuO/ SrTiO₃(001).

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