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Growth, structure and defects in GeTe thin films grown on silicon substrates: the key role of atomic steps

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Ferroelectric Rashba semiconductors are a novel class of materials with strong potential for spintronic applications [1,2]. For GeTe thin films, as a prototype of this class of materials, it has been shown that the ferroelectric polarization can be reversed in an electric field [3], and the spin chirality of the band structure is consistently changed [4].

We have grown and characterized GeTe thin films on Si(111) single crystal by Molecular Beam Epitaxy (MBE) [5]. In this presentation I will first address the structure and morphology of GeTe thin films during the early stages of growth [6]. Using scanning tunneling microscopy (STM) we show that GeTe thin films grow initially via a homogeneous and crystalline buffer layer. Then atomically flat 2D islands of GeTe nucleate and grow preferentially at Si step edges. An interfacial relaxation mechanism occurs via threading dislocations (Frank-Read sources) that promotes a layer-by-layer growth mode. This process is rapidly dominated by a step-flow growth mode of GeTe layers. Despite a high surface morphology quality, a significant amount of mirror domains and in-plane misorientations between adjacent grains is evidenced by low energy electron diffraction (LEED) and dark-field low energy electron microscopy (LEEM). These defects are buried close to the interface with the Si substrate and strongly decay with the film thickness.

Considering the key role of atomic steps in the growth process, we have proposed to use miscut substrates to suppress interfacial defects. In that perspective we have grown GeTe films by MBE on vicinal Si substrates with a miscut angle between 2° and 10° with respect to Si(111) substrate. The morphology, structure and ferroelectric state has been characterized by x-ray diffraction, TEM, SEM and LEEM. The role of the miscut angle on the growth is clearly evidenced: most interfacial defects can be suppressed. In addition since ferroelectricity and ferroelasticity are intimately related properties in GeTe thin films, the stress relaxation mechanisms at GeTe/Si interface via atomic steps can favor one type of ferroelastic/ferroelectric domain. At last the size decay of ferroelectric domains during annealing is attributed to thermo-mechanical stresses arising from the significant difference of linear thermal expansion coefficients of Si and GeTe [7].

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Engineering of diamond growth for quantum applications

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The development of applications in quantum sensing requires dedicated solid-state material platforms with unprecedented control over quality, purity and doping. Indeed, Quantum Technologies explore our ability to coherently control the peculiar properties of nanoscale quantum systems and harness their potential in a wide range of fields including health, communications, security and environment.

Atomic-scale defects in solid-state materials are among the most promising candidates and several platforms are being considered such as donors in silicon, color centers in semiconductors, rare-earth ions in oxides, quantum dots etc. One of the inherent drawbacks of the extreme sensitivity of such spin systems to the field they are supposed to measure, is the necessity to carefully control their close crystalline environment in order to maximize coherence properties which pushes the fabrication technologies to their limits. In this presentation, we will review the main challenges in the synthesis of suitable "quantum-grade" diamond materials using color centers and more specifically NV centers. Issues related to the control of their density and the maximization of their coherence properties through precise engineering of the growth process will be discussed. (i) Atomic scale defects need to be introduced on demand within diamond. High amounts are usually preferred in most sensing schemes but limits exist in the ability to control growth at high doping levels as well as to avoid interaction between nearby spins. (ii) Nuclear spins within the matrix itself might cause decoherence and growth of isotopically enriched materials allows considerably extending T2 times. (iii) In a similar way, magnetic sensitivity of a sensor based on NV ensembles can be considerably increased by producing diamond with NV centers having preferential orientation which can be obtained by using diamond substrates with specific crystallographic orientation (iv) Controlling the spatial localization of color centers is crucial to the sensing device since their interaction strongly depends on the distance to the field that is to be sensed. (v) Controlling the shape and the size of the diamond platform remains also a very challenging point.

Epitaxial two-dimensional transition metal disulfides

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Chalcogen atoms have strong affinity with transition metals (and copper in particular, therefore the greek etymology of the word), forming a variety. Among these alloys are lamellar compounds, some of which are found in nature. Specifically, transition metal *dichalcogenides* can be obtained in the form of single layers each consisting of a chalcogen / transition metal / chalcogen sandwich. Their unique, in some cases strongly spin-polarized, two-dimensional electronic properties, give rise to exciton-driven light emission at room temperature, charge-ordered quantum states, so-called charge density waves influenced by electron-electron interactions; these compounds may also host desirable ferroic states (ferromagnetism, ferroelectricity). The range of possible properties further extends when stacking the single-layers to assemble van der Waals heterostructures.

The first transition metal dichalconides to be isolated as a single-layer were disulfides — MoS_2 was mechanically exfoliated in 2005, using scotch tape, and again in 2010-2011 to unveil exceptional optoelectronic properties. Alternative approaches to this mainstream production method exist. Among them is epitaxial growth, first demonstrated in year 2000 (again, with MoS_2). Such a method yields films fully-covering their substrate (unlike mechanical exfoliation). Whether bottom-up growth can deliver layers of precisely controlled thickness and with domain size beyond 1 µm remains, however, an open question.

We operate a ultra-high vacuum system, combining *molecular beam epitaxy* and *pulsed laser deposition* capabilities with advanced characterization tools (electron diffraction, Auger electron spectroscopy, scanning tunneling microscopy, Raman scattering / photoluminescence spectroscopy at variable temperature). Using this multi-technique system, we grow single-layers of MoS_2, TaS_2, and FeS_2, which are appealing for their excitonic, charge-order, and ferromagnetic properties respectively. The stoichiometry and crystallography of these three disulfides are more-or-less easy to control — the sought-for forms may for instance differ from those of the known three-dimensional, naturally-occurring minerals. On a substrate, the 2D materials exhibit a spatial modulation of their structure as they form moiré patterns. A very high structural quality can be obtained in some cases, as shown by high-resolution synchrotron X-ray diffraction performed in a collaboration with colleagues from CEA-MEM (Gilles Renaud and coworkers).

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Title : Two dimensional electron gases to investigate exotic electronic excitations

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Two-dimensional electron gases (2DEGs) in GaAs-based heterostructures is the constituent of choice for a number of quantum circuits. They have allowed novel studies of exotic electronic excitations emerging in presence of strong Coulomb interactions. These includes investigations of anyonic properties in the fractional quantum Hall effect (fractional charges, anyonic statistics as well as scaling dimensions) and of exotic quantum critical points resulting from frustrated Kondo interactions.

In this talk, we will discuss the realisation of the III-V heterostructures and devices, and the strategies developed to achieve the necessary properties of the 2DEGs as well as the components of the devices (quantum point contacts, screening gates, ohmic contacts) to conduct these studies. We will focus on an exemplar experiment where we measured entropy of an exotic excitation, detailing the quantum circuit step-by-step.

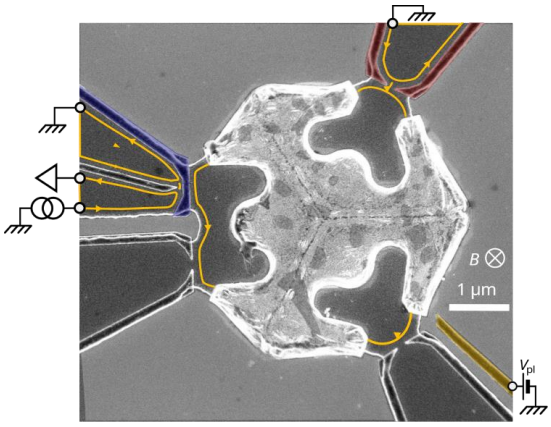

Fig.1. Metal-semiconductor charge Kondo device with a charge sensor to measure entropy.

Epitaxy-tuning of the magnetic properties of Mn_5Si_3 thin films: from antiferro- to alter-magnetism

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For many years, the anomalous Hall was believed to be exclusively present in ferromagnetic materials. However, it has been recently shown that these effects can be finite also in certain collinear antiferromagnets displaying a specific crystal and spin symmetry, which tremendously broadens the pool of materials in which spontaneous Hall is expected [1].

Here, we report on a route to grow epitaxial Mn_5Si_3 thin films on Si(111). To this end, we use Mn and Si codeposition in a molecular beam epitaxy system, and carefully tune the deposition rates, the growth temperature, and the annealing temperature. The silicide phase-formation and morphology are assessed using reflection high-energy electron diffraction, X-ray diffraction, high resolution transmission electron microscopy and atomic force microscopy. We show that it is possible to grow high quality crystalline Mn_5Si_3 thin films using interface engineering by means of a thin interfacial MnSi layer (Fig.1a) [2]. The Mn_5Si_3 crystalline quality is intimately related to MnSi strain-state that can be tuned with growth parameters. Unlike bulk or polycrystalline films, our films exhibit an altermagnetic behavior (Fig.1b, Fig.1c) [3-6] that is highly sensitive to the Mn concentration and the crystal quality, highlighting its electronic band-structure origin.

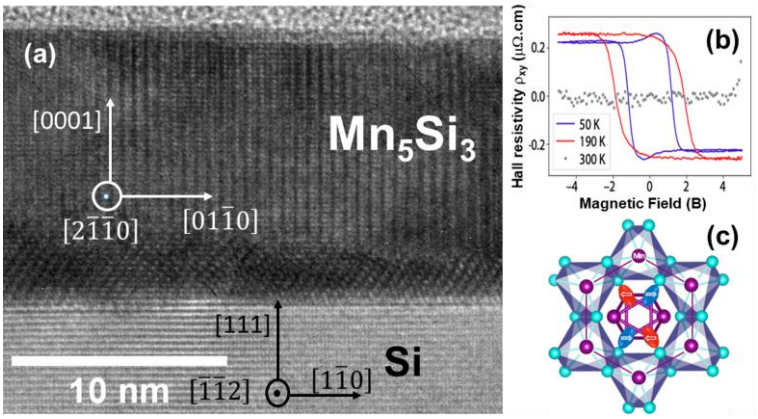

Fig. 1: (a) High-Resolution TEM cross-section of a 13-nm thick Mn_5Si_3 thin film grown on Si(111). (b) Anomalous Hall resistivity in the antiferromagnetic phase measured at 50 K, 190 K and 300 K. (c) Magnetic and crystalline structure of Mn_5Si_3.

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Epitaxy of group-IV semiconductors for quantum electronics

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Epitaxy of group-IV semiconductors is a key enabler for quantum devices. Low temperature epitaxy can be used to deposit Si:B layers with boron concentrations so high that they are superconductive (ECS Transactions 98 (5), 203 (2020)). Tensily strained Si layers sandwiched between relaxed $Si_{0.7}Ge_{0.3}$ layers behave as quantum wells for electrons, enabling electron spin quantum bit (qubit) fabrication. Purified ^{28}Si without deleterious ^{29}Si isotopes (with a nuclear spin) are ideal as the core of fully-depleted, multiple gate transistors for qubits. Compressively-strained Ge layers sandwiched between relaxed $Si_{0.2}Ge_{0.8}$ layers can confine a two-dimensional hole gas (2DHG) offering an emerging pathway to hole-spin qubits.

In the following, we will focus on the latter two subjects. We will show how we succeeded in growing ^{28}Si layers with the following concentrations: ^{28}Si isotopes > 99,992%, ^{29}Si isotopes < 0.006% and ^{30}Si isotopes < 0.002% (Journal of Crystal Growth 509, 1 (2019)). Such values can instructively be compared to those in natural Si: ^{28}Si: 92.223%, ^{29}Si: 4.678% and ^{30}Si: 3.092%. The availability and cost of isotopically enriched $^{28}SiH_4$ is a major difficulty, however. We thus quantified the impact of growth temperature and HCl mass-flow on the Si growth rate. At high temperature, above 850°C, we reached a silane supply limited regime with a good decomposition efficiency, high growth rates (> 100 nm $min.^{-1}$ for the SiH_4 mass-flow selected) and almost no impact of the HCl flow. There was otherwise, below 850°C, a H- and Cl-surface desorption limited regime, with a lesser decomposition efficiency and Si growth rates which dropped as the temperature decreased and/or the HCl mass-flow increased. Thick ^{28}Si layers should be grown at high temperature, while low temperature epitaxy should be limited to the deposition of thin ^{28}Si layers on top of SiGe sacrificial layers (^{28}SOI fabrication with a bonding-etch back approach) or the thickening of SOI substrates (to avoid elastic or plastic relaxation/dewetting).

We otherwise fabricated c-Ge/SiGe heterostructures for hole spin qubits. We first grew at 850°C, 20 Torr and with a $SiH_2Cl_2 + GeH_4$ chemistry, SiGe virtual substrates (VS), with a gradual ramping-up of the Ge concentration (to confine misfit dislocations) and a capping with 3 µm thick constant composition layers. Reciprocal Space Maps around the (004) and (224) X-Ray Diffraction (XRD) orders gave us the Ge concentration in those SiGe caps (73.8% and 78.7%) and their macroscopic degrees of strain relaxation (102.0 and 102.5%). The surface cross-hatch, e.g. the regular array of undulations with a 1-2 µm spatial wavelength because of a periodic strain field in VS, was suppressed using Chemical Mechanical Polishing (CMP). We then grew on top of the polished SiGe VS, at 500°C, 20 Torr and with a $SiH_2Cl_2 + GeH_4$ chemistry, {100 nm thick SiGe 74% or 79% / 16 nm thick compressively-strained Ge / variable thickness SiGe 74% or 79% overlayer / Si 2nm cap} stacks. The parameter that changed was the SiGe overlayer, with 22, 33, 44 or 55 nm thicknesses probed.

Compared to polished surfaces, a slight surface roughening was observed for the SiGe stacks, larger for the SiGe 74%/c-Ge than for 79%/c-Ge stacks. Thicker SiGe overlayers yielded smoother surfaces. We ascribe these surface undulations, with a ~ 100 nm wavelength, to an elastic relaxation of the compressive strain in the c-Ge layers. XRD showed that those stacks were pseudomorphic, with the same in-plane lattice parameter for the c-Ge layers than that of the SiGe VS underneath. Energy Dispersive X-ray spectroscopy (EDX) mapping of the whole structure showed that the Ge grading was rather linear with, as intended, a 10% Ge/µm grading. Cross-sectional Transmission Electron

Microscopy (TEM) showed the presence of numerous misfit dislocations in the graded layer and none in the thick $Si_{0.21}Ge_{0.79}$ / c-Ge stack on top. A slight Ge concentration increase, by a few %, was measured by EDX at the CMP location, with a perfect crystallinity in the stack grown on top. The 16 nm thick c-Ge layer itself was perfectly monocrystalline, with a 1-2 bi-atomic layer roughness at c-Ge/SiGe interfaces, no in-plane deformation compared to the surrounding SiGe and an out-of-plane deformation of 1.5% from Precession Electron Diffraction.

Magnetotransport measurements in Hall-bar devices were performed at 4.2 K to assess the electrical properties of the 2DHG in the grown SiGe/c-Ge heterostructures. At low magnetic field, a hole mobility of 1.2 x 10^5 cm^2 V^{-1} s^{-1} was obtained for a hole density of n_{2DHG} = 3.7x10^{11} cm^{-2} in the c-Ge/SiGe 79% 55nm sample, whereas quantum Hall effect plateaus and Shubnikov-De-Haas oscillations were observed at higher fields (ECS Transactions 111 (1) 53 (2023)).

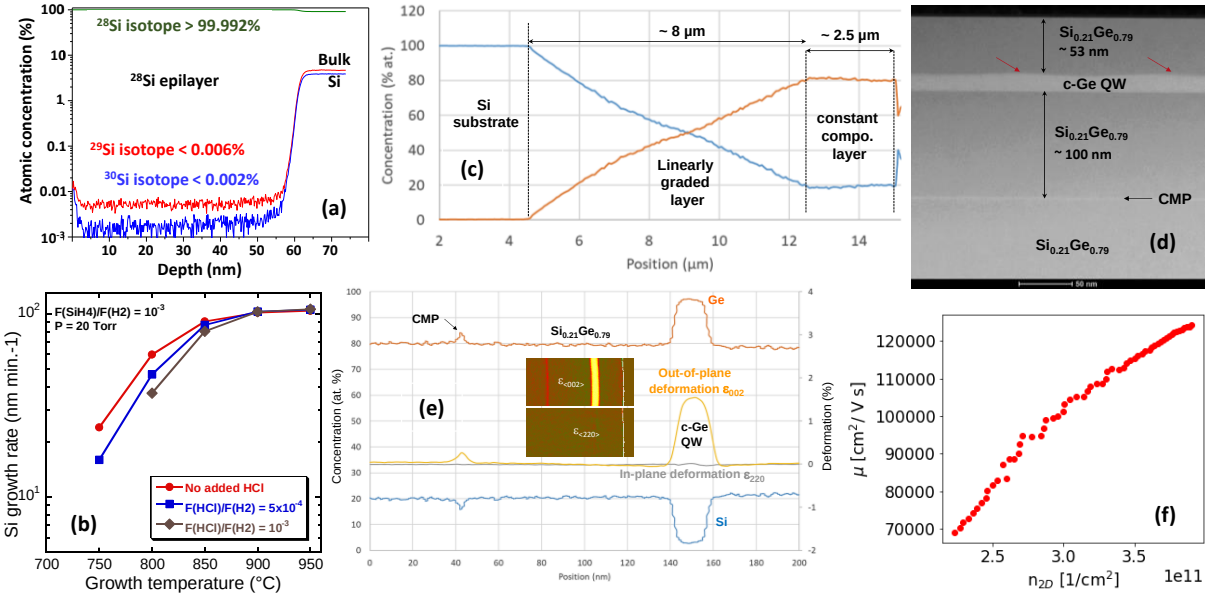

Figure 1 : (a) SIMS depth profiles of Si isotopes in a ^{28}Si epilayer; (b) Si growth rate function of the growth temperature and HCl flow for a given SiH_4 flow; (c) EDX profile of the Ge and Si concentration in a $Si_{0.21}Ge_{0.79}$ virtual substrate; (d) SiGe/c-Ge/SiGe/Si cap stack grown at 500°C on a polished $Si_{0.21}Ge_{0.79}$ virtual substrate; (e) Ge and Si concentration & deformation depth profiles in that 2DHG heterostructure; (f) mobility @ 4.2K function of the 2DHG sheet density.

Bismuth-based topological insulators for quantum computing and spintronic applications

Topological insulators (TI) are functional materials holding unique promises for future quantum computing and spintronic applications. Indeed, their topologically protected surface states (TSS) can be advantageously combined with superconductors or magnetic materials for creating new hybrid interfaces. In this context, we present the epitaxial integration of Bismuth-based TI on industrial substrates by molecular beam epitaxy, their structural and electrical characterizations, and demonstrate the presence of the TSS [1-3]. Both, superconductors and magnetic materials can be integrated on these TI for realizing hybrid interfaces and a few examples will be presented. In the latter case, the electrical switching of a Cobalt layer presenting a perpendicular magnetic anisotropy (PMA) is demonstrated [4].

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Rare Earth-Diamond Hybrid Structures for Optical Quantum Technologies

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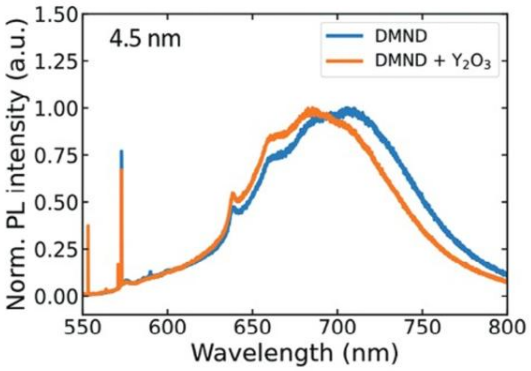
Associating distinct quantum centers in a hybrid structure can achieve new functionalities providing that the underlying properties of each component are preserved. In this work, we combine two systems with outstanding optical and spin properties that have been broadly used for quantum applications such as sensing and communications: NV^- color centers in diamond [1] and rare earth (RE) doped crystals [1,2].

The hybrid structure consists of a rare earth doped Y_2O_3 thin film deposited by direct liquid injection chemical vapor deposition (CVD) on a single crystalline diamond substrate in which shallow NV^- were implanted [3]. We investigated in detail the structure of the films and the optical and spin properties of rare earth ions and NV^- centers. Photoluminescence decays of the Er^{3+} telecom wavelength $^4I_{13/2}$-$^4I_{15/2}$ transition measured at room and low temperatures indicate a low concentration of defects in the films, with lifetimes up to 16 ms, whereas high-resolution spectroscopy reveals inhomogeneous broadening comparable to that reported on films deposited on other substrates like silicon. In addition, optical and spin properties of the NV^- before and after Y_2O_3 thin film deposition show they are not strongly affected by the film deposition. These promising results [4] suggest that the proposed structure can be useful for integrating the rare-earth ions with NV^- centers at the nanoscale level for developing hybrid solid state quantum systems.



Emission spectrum of NV^- centers implanted at a depth of 4.5 nm in diamond (blue). Deposition of a Y_2O_3 thin film preserves emission properties (orange).

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III-Sb based semiconductors and heterostructures

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Among the III-V compounds the so-called “antimonide-based compound semiconductors” (III-Sbs) are the compounds which can be grown on a GaSb substrate. This includes GaSb, InAs, InSb, AlSb and their alloys. III-Sbs exhibit unique properties among semiconductors:

- Their natural bandgaps cover the whole range from 0.15 eV to 2 eV, *i.e.* the whole near infrared (IR) to long IR range.
- Band offsets in the conduction and valence bands cover the 0 – 2 eV and 0 – 0.5 eV, respectively.
- Band alignments exist in all possible configurations: type-I, type-II or type–III.
- Their carrier effective masses/mobilities are the lightest/highest of all III-V compounds.

These properties offer unrivalled opportunities for extensive band-gap and band-offset engineering, and for device design. In particular they allow creating artificial, man-made materials whose effective bandgap can be varied by design in the whole range from the near-IR to the long-IR. The III-Sbs are well suited to develop a number of devices such as high frequency transistors, IR lasers, imaging IR photodetectors. In this talk, I will first introduce the III-Sbs technology and review its peculiarities in terms of epitaxy. Then, I will summarize recent achievements in mid-IR optoelectronics, and show how this technology allows investigating topological states.

Development of superconductor-semiconductor nanowires for quantum circuits

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The epitaxy community is making significant advances in high-quality superconductor-semiconductor hybrids. These heterostructures hold promise for enabling error-limited quantum computation through qubits with longer coherence times, as well as topologically protected qubits. This effort began with the quest for improved material interfaces for gate tunable Josephson junctions, such as optimized Al/InAs and Al interfaces. However, aluminum is limited in terms of critical current, and many other superconductors remain underexplored.

Here, we present our efforts to develop expertise in large supercurrent nanowire Josephson junctions either by using parallel Al/InAs nanowires or by using an alternative superconductor such as tin (Sn). Tin is known for having higher critical temperatures (Tc) and higher superconducting gap than aluminum. However, it is an allotrope, meaning it can exist in multiple crystalline phases, with only one phase being suitable for quantum bit technologies. Therefore, significant work is needed to control the crystalline phase of Sn during epitaxy or deposition to favor the desired phase [1,2]. Additionally, it is critical to ensure that interfaces remain undamaged during the growth process.

Both our strategies show large improvement and tunability of the critical current. In the case of Sn/InAs nanowires, the devices show additionally strong resilience to magnetic fields [3]. Tunable and large critical currents as well as magnetic field resilience are essential properties for quantum devices. Preliminary measurements of Josephson parametric amplifiers and gatemon qubits will be presented.

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Substrate matters - how the properties of the lamellar topological insulator Bi_2Se_3 depends on the substrate-epilayer interface.

(and a brief overview of the MBE facility at the INSP)

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The MBE facility at the INSP consists of a stand-alone arsenides MBE machine (fig. 1a) and a cluster of two chalcogenides MBE machines, and STM, XPS and metals chambers (fig. 1b).

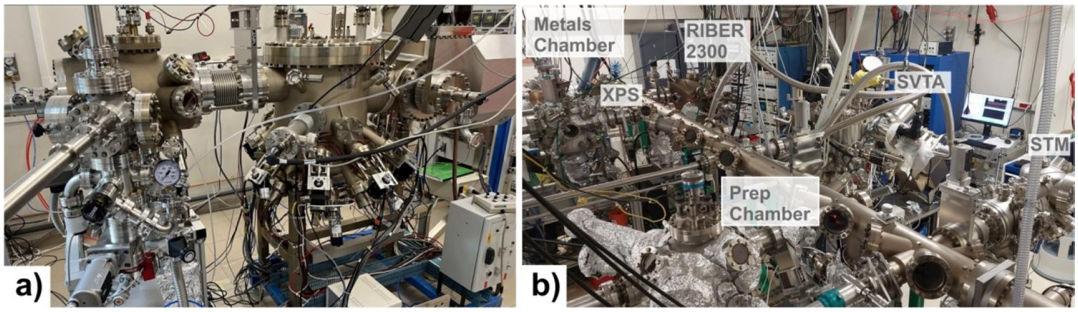

Fig 1 a) Arsenides MBE: a modified RIBER C21 designed for both RHEED and grazing-incidence fast atom diffraction measurements, currently used for the growth of GaAs/AlAs , InAs/GaAs quantum dot devices, **b)** Chalcogenides MBE cluster : equipped for the growth of transition metal dichalcogenides, II-VI, III-VI and IV-VI materials (selenides and tellurides).

After a brief overview of the ongoing projects at the MBE facility at the INSP, we will discuss the growth and properties of the lamellar topological insulator Bi_2Se_3.

Topological insulators (TIs) are characterized by both a bulk energy gap and metallic surface states that are spin-momentum locked. The bulk bandgap of Bi_2Se_3 (~220 meV) is relatively large compared to other TIs. This, together with the fact that the Dirac crossing point of the metallic surface states lies within the bulk band-gap, makes it appear an attractive material for room temperature spintronic devices based on transport in the TI metallic states.

However the high density of native defects such as Se vacancies in Bi_2Se_3 leads to a highly n-type bulk material, instead of an insulating bulk material, despite the large energy gap. In addition to these native charged defects, the bulk carrier density of thin films is also affected by the presence of twin-defects and downward band-bending both at the substrate-epilayer interface and the epilayer surface. Here we will discuss the effect of growth conditions, substrate choice and substrate preparation on the film structural, optical and transport properties and how a combination of strategies can be used to reduce the bulk carrier contribution.

Tuning Silicon and SiGe superconductivity with Nanosecond Laser Doping

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Since the discovery of BCS superconductivity in silicon by nanosecond laser ultra-doping with boron, theoretical and experimental works have endeavoured to understand what triggers and controls the superconducting phase. Indeed, superconducting Si has great potential to develop a cryogenic electronics with the advantages of large scale integration and high reproducibility. Through the optimization of the nanosecond laser temporal profile, we achieved an excellent control of both the electrical and structural properties of ultra-doped Si thin layers, with a maximum carrier concentration of 8 at.%, 5 times higher than the state of the art, in monocrystalline epilayers with no defects, 100% dopant activation up to and above the solubility limit, and homogeneous doping profile [1-3].
The control and improvement of the active doping is directly reflected in the control of the superconducting critical temperature Tc of such disordered superconductor, increased by 30% in this optimized setup, in agreement with theory and opposite to previous results (Fig.1) [2].
Furthermore, we demonstrated that superconductivity is not only controlled by doping, but also by the lattice deformation. Thus, it is possible to tune up to 50% Tc by modifying by 1% the lattice parameter, as shown through nanosecond laser incorporation of Ge up to 20 at.% [4].
Mastering and understanding the materials properties has brought to the development of all-silicon devices, such as Josephson junctions and superconducting microwave resonators [3].
Indeed, SQUIDs and Josephson junctions were developed [5], thanks to the excellent, epitaxial, transparent interface between superconducting Si and semiconducting Si. Finally, to explore the dynamics of superconducting Si, we realised microwave silicon resonators (f~1-10 GHz, Q~4000) [6]. We have shown a strong non-linear response with power, observing a Kerr coefficient ~300 Hz/photon where less than 1 Hz/photon was expected. This suggests that, once the losses sources identified and reduced, silicon resonators may be promising candidates for on-chip strongly non-linear quantum devices.

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Building Quantum layer by layer with III-V

Molecular Beam Epitaxy (MBE) has played a pivotal role in advancing quantum optical materials since its invention in the 1960s. Epitaxy refers to the precise deposition of crystalline thin layers on a substrate, ensuring that the deposited material inherits the underlying crystal structure. MBE, in particular, allows for atomic-scale control over material composition and layer thickness. This technique has enabled the fabrication of high-quality semiconductor heterostructures essential for mesoscopic physics and quantum optics. I will give a brief historical review of this technique in the first part.

One of the most significant achievements of MBE is the growth of III-V heterostructures, which serve as the backbone for many quantum devices. As an example, I will discuss about InAs quantum dots embedded in a GaAs matrix, which exhibit discrete energy levels as "artificial" atoms. These quantum dots are excellent deterministic source of single-photon. This property makes them ideal for quantum cryptography and quantum computing, where secure communication and qubit implementation require highly coherent single-photon sources.

As a second example, I will show how we can create polaritons, which are hybrid light-matter quasiparticles formed through the strong coupling between excitons and cavity photons. These polaritons serve as a platform for quantum simulation, enabling the exploration of many-body quantum physics, non-equilibrium phase transitions, and topological states of light

Anomalous dynamical dewetting of silicene flakes with dendritic pyramids

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The production by exfoliation of two-dimensional (2D) materials has opened up a fertile field of study, enabling their integration into a variety of structures for different materials. However, their production by epitaxy, which is a priori more controlled, remains largely to be developed and mastered. This is the case in general, and in particular for systems such as silicene, which cannot be produced by exfoliation. Group IV elements such as Si (silicene) and Ge (germanene) are indeed promising alternatives, that are predicted to be Dirac materials in which electrons behave as relativistic massless particles. Numerous attempts to grow silicene have been made on different metallic or van-der-Waals substrates, with varying degrees of success in terms of the reality, quality and size of the 2D Si layer thus produced. A natural option is therefore to introduce a buffer vdW layer for decoupling the 2D adlayer from its substrate. Recent experiments reported the possibility to grow silicene on a high quality graphene grown by CVD on a 6H-SiC(0001) substrate. They demonstrated the possibility to grow large silicene flakes over 100nm in size. Yet, they follow an anomalous growth mode that is not described by conventional epitaxial growth models, and needs better control.

We will review the experimental growth of silicene on a vdW substrate. We will detail the particular aspects of this growth, its strengths and limitations. We will then show how this growth can be modeled thanks to a dynamical modelization. A lattice-based model will be introduced derived that revisits the dewetting thermodynamics and considers generally ignored adsorption and step-edge energies. It is investigated using kinetic Monte-Carlo simulations and mean-field rate equations, and implemented by close inspection of microscopy images. This process unveils an anomalous growth mode that reproduces the morphology of the flakes and their dynamical evolution, and provides guidelines on experimental conditions for high-quality silicene growth.

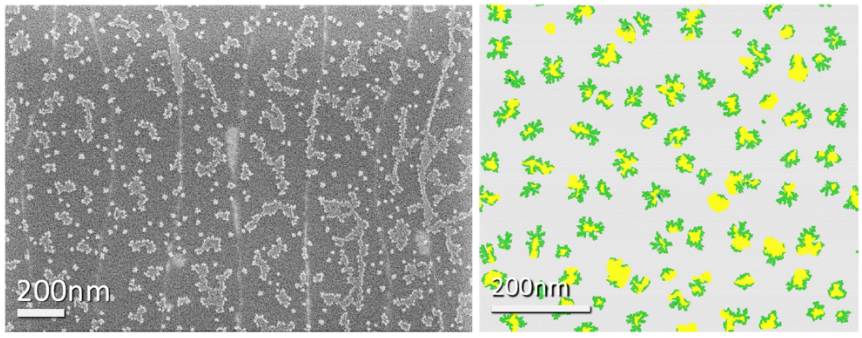

Figure 1: (left) silicene flakes on Gr ; (right) kinetic Monte-Carlo simulation of silicene growth

Study of electrically active defects in fully depleted silicon-on-insulator transistors designed for hole spin qubits

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Silicon holds significant potential as a material for future quantum processors. Transistors built on a silicon-on-insulator template functioning as silicon quantum bit (qubit) devices can be fabricated using industry-standard processes, allowing for easy integration with classical control hardware [1]. However, achieving precise management of carrier transfer within the transistor channel is essential, requiring the elimination of electrically active defects that could act as recombination centers. Optimizing such a device demands a detailed characterization of the channel to assess the material purity.
This study examines the presence of defects in the channel of fully depleted silicon-on-insulator transistors designed for qubit applications. The ON state of the transistor is achieved by applying a negative voltage to the gate. Source and drain electrodes were connected together and voltage pulses were applied to the gate contact to perform capacitance deep level transient spectroscopy (DLTS) measurements between 77 K and 350 K. Electrical simulations conducted using Sentaurus device simulator showed that a depleted section of the channel extends beneath the gate and towards the source and drain regions when applying a positive voltage to the gate contact. By adjusting the positive reverse bias and applying negative voltage pulses, we were able to probe the channel and localize the electrical active defects responsible for the DLTS signal.

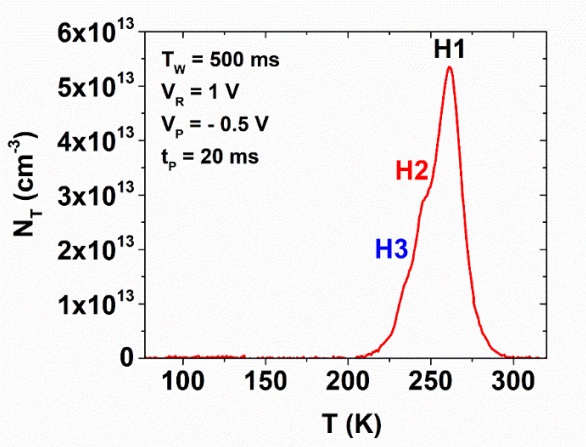

Figure 1: Capacitance DLTS spectrum of the fully depleted silicon-on-insulator transistors. The detection of three hole traps labeled H1, H2 and H3 reveals the presence of electrically active defects in the probed zone located in the onset of the implanted regions.

Three dominant hole traps were detected (figure 1) at respectively 0.54 eV, 0.57 eV and 0.65 eV above the valence band edge in the source/drain regions and are associated with bulk [2] and Si/SiO_2 interface defects [3]. Their origin is likely related to the damage produced during the formation of the p-doping by implantation. This study highlights the high quality of the channel material below the gate stack but also the need to keep the source and drain regions far from the gate edges to improve the qubit stability.

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Tuning Silicon superconductivity with nanosecond laser doping

L. Desvignes[1], D. Débarre[1], G. Hallais[1], L. Largeau[1], G. Priante[3], M. Amato[4], A. Debernardi[2], and B. Sermage[3] and F. Chiodi[1]

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Since the discovery of BCS superconductivity in silicon by nanosecond laser ultra-doping with boron, multiple theoretical and experimental works have endeavored to understand what triggers and controls the superconducting phase. Indeed, superconducting Si has great potential to develop a cryogenic electronics with the advantages of large scale integration and high reproducibility. Through the optimization of the nanosecond laser temporal profile, we achieved an excellent control of both the electrical and structural properties of ultra-doped Si thin layers, with a maximum carrier concentration of 8 at.%, 5 times higher than the state of the art, in monocrystalline epilayers with no defects, 100% dopant activation up to the solubility limit, and a homogeneous doping profile [1-3]. Moreover, we demonstrated that the carrier concentration attained is the maximum that could be achieved: at such large doping concentrations, the concentration of substitutional, active, single B atoms is 'geometrically' limited by the non-negligible probability of having a substitutional B neighbor, thus creating an inactive dimer (Fig 1a) [2]. The control and improvement of the active doping is directly reflected in the control of the superconducting critical temperature Tc, increased by 30% in this optimized setup, in agreement with the theoretical expectations as opposite to previous results (Fig.1b) [2]. Furthermore we demonstrated that superconductivity is not only controlled by doping, but also by the structural properties, and in particular the lattice deformation: on one side, the superconductivity threshold corresponds to the relaxation of the doping-induced strain, and on the other, it is possible to tune up to 50% the Tc by modifying by 1% the lattice parameter, as shown through nanosecond laser incorporation of Ge up to 20 at.% [4].

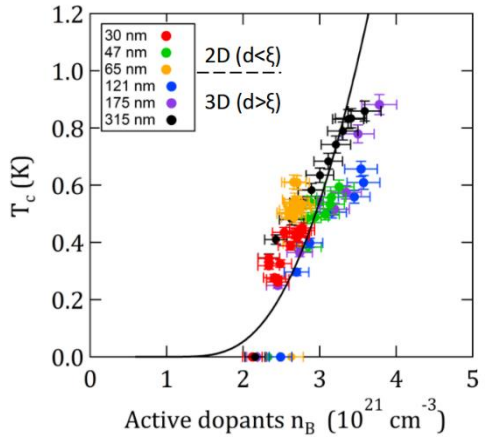

Fig 1: b) Superconducting critical temperature vs active B concentration of thin SiB layers 30 to 175 nm thick, superposed to the theoretical expectations (theory adapted from Boeri, PRL 2004)

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Inverse Rashba Edelstein THz emission modulation induced by ferroelectricity in van der Waals heterostructures

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Spintronic Terahertz emitters, based on optically triggered spin-to-charge conversion (SCC) processes, have recently emerged as novel route towards compact and efficient THz sources. Yet, the next challenge for further technologically-relevant devices remains to modulate the emission, with low-energy consumption operation. To this aim, ferroelectric materials coupled to active spin-orbit layers such as two-dimensional transition metal dichalcogenides are potential candidates. In this work, we present the realization of a large area heterostructure of CoFeB/$PtSe_2$/$MoSe_2$ on a bidomain $LiNbO_3$ substrate and propose to elucidate the SCC mechanisms at work using THz time-domain spectroscopy together with density functional theory calculations.

Samples were first prepared from a $LiNbO_3$ wafer with pre-poled out-of-plane polarization areas along opposite directions, and cut into 10x10 mm^2 coupons, with half the area hosting a polarization pointing up (up area) and half pointing down (down area). The 2D layers constituting the $MoSe_2$/$PtSe_2$ van der Waals heterostructure were grown using molecular beam epitaxy on a Mica substrate and transferred onto the ferroelectric substrate in an aqueous environment [1]. Finally, a 3 nm-thick ferromagnetic layer made of CoFeB was deposited by sputtering without breaking vacuum, followed by 4 nm of Al to prevent oxidation, defining the heterostructure depicted in Fig. 1a.

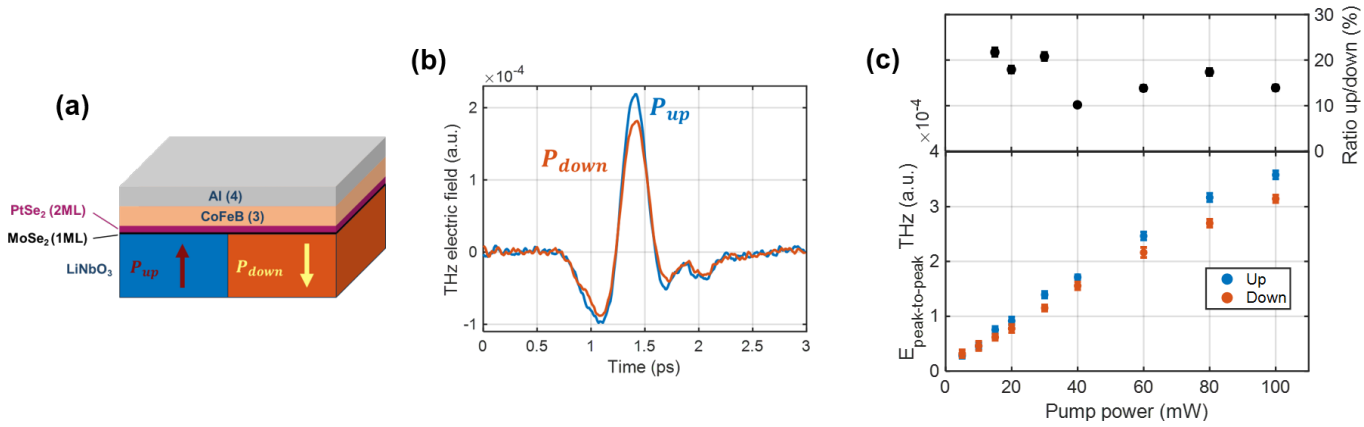

Figure 1: (a) Schematic of the full heterostructure. Numbers in parentheses express the number of monolayers (thickness in nm) for 2D (bulk) materials, respectively. (b) Temporal traces of magnetic THz contribution for up and down areas. (c) Down panel: Peak-to-peak amplitude of the magnetic contribution for up and down areas, as a function of the incident infrared pump power. Upper panel: Calculated ratio between the peak-to-peak amplitudes in up polarized and down polarized areas in % (ratio up/down) as a function of incident pump power.

The THz emission properties of the system were probed using standard THz time-domain spectroscopy technique in transmission mode. Samples were excited from the substrate side ($LiNbO_3$) at normal incidence by linearly polarized 80 fs-long pulses centered at 800 nm (photon energy ∼1.55 eV) while applying a small in-plane magnetic field (∼20mT). We probed up and down ferroelectric areas for two opposite directions of the magnetic field, allowing to extract the magnetic

contribution to the THz emission by performing the difference of the time traces [2]. We observe that both THz signatures are of the same positive phase, with a sizable increase of the THz emission in the up-poled area compared to the down one (Fig. 1c). This result shows that the ultrafast spin current generated in the FM layer under illumination is efficiently converted into a charge current into adjacent layers, in the vicinity of $LiNbO_3$/2D interface. Interestingly, we also observe that the THz emission remains always higher for the up area over a large range of pump power excitation (see Fig. 2a) corroborating the influence of ferroelectricity direction on SCC efficiency. We evaluate the induced ferroelectric modulation on SCC to be about 15-20%.

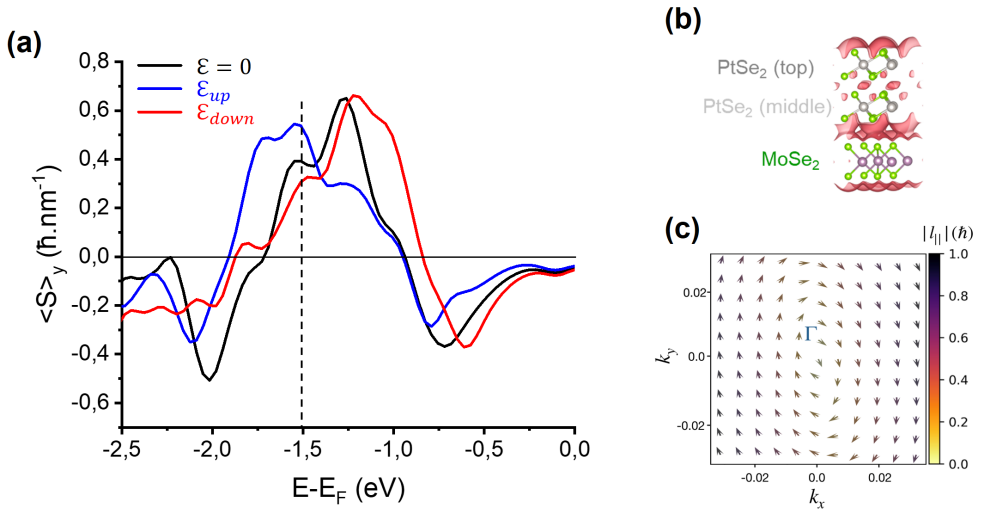

Figure 2: (a) Spin accumulation as a function of the energy for the trilayer, at equilibrium (black) and while applying an external electric field $\mathscr{E}$=0.25 V/Å pointing up (blue) and down (red). (b) Charge density for the trilayer at the isosurface 0.01 e/Å^3, displaying the strong hybridization between $MoSe_2$ and $PtSe_2$. (c) Spin texture at an energy cut of E=E_F-1.5 eV (vertical dashed line in (a)) showing Rashba states.

We now turn to Density Functional Theory of SCC phenomena in these systems. We evaluate in Fig. 2a the spin accumulation response, related to the Rashba Edelstein tensor and thus THz emission, at equilibrium and for an electric field $\mathscr{E}$ pointing either up or down, in agreement with our experiment. In the absence of any additional polarization field ($\mathscr{E}$=0), a strong and positive spin accumulation is observed in the valence band. In the presence of an electric field pointing up (down), the spin accumulation remains positive and is shifted towards lower energy (higher energy), resulting in a total energy shift of about 0.32 eV, in agreement with previous experimental observation in similar systems [1]. At an energy cut of E=E_F-1.5 eV (vertical dashed line in Fig. 2a), corresponding to the photon energy of our pump laser, the spin up accumulation becomes larger than the down one, in qualitative agreement with our experimental results. The charge density map (Fig. 2b) highlights the conversion location in the heterostructure, showing a strong hybridization between $MoSe_2$ and $PtSe_2$ layers. Since $MoSe_2$ takes part to the inversion symmetry breaking, it lifts the degeneracy present in $PtSe_2$, leading to Rashba states (Fig. 2c) as already reported in the case of $PtSe_2$/Gr bilayers [3], in which SCC also occurs in the valence band. We thus interpret the observed THz emission change in up and down areas to arise from SCC mediated by Inverse Rashba-Edelstein effect at the interface between $MoSe_2$ and $PtSe_2$, and modulated by ferroelectricity..

Acknowledgments

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