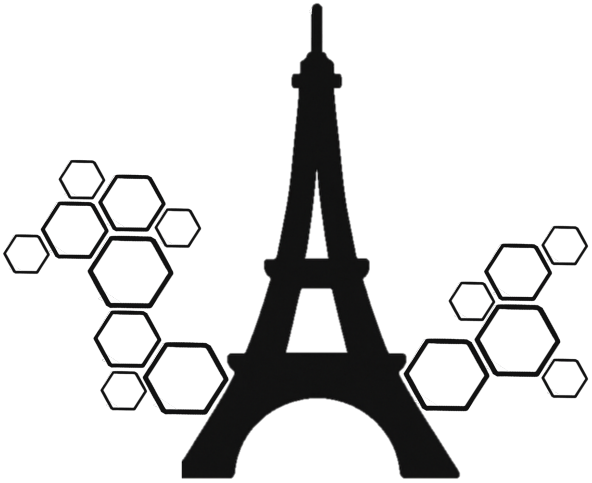
3rd International Workshop

Hexagonal SiGe and Related Materials



27-28 October 2025

International Conference Center
Sorbonne Université
Paris, France

Organizers

Michele Amato
Université Paris-Saclay, France

Silvia Pandolfi
Sorbonne Université, France

Silvana Botti
Ruhr University, Germany

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https://workshop-hexsige-2025.github.io/

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Venue

International Conference Centre Sorbonne Université (CICSU)
Patio 44, 4
Place Jussieu 55, 75005 Paris, France

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1. Description

The 3rd International Workshop on Hexagonal SiGe and related materials will take place on **27-28 October 2025** at the International Conference Center of **Sorbonne Université in Paris, France**. The key objective of this interdisciplinary workshop is to identify challenges towards a fundamental understanding of the main properties of hexagonal silicon and related materials. This will be the third edition of a series of workshops on the physics, chemistry and applications of group IV hexagonal materials after the two successful previous editions in Eindhoven (2023) and Milan (2024). By bringing the most recent experimental and theoretical viewpoints together, we aim to cover the following topics:

- Growth of Hex-SiGe nanowires.
- Planar growth of Hex-SiGe and integration on silicon.
- Characterization of structural, electronic, and optical properties of Hex-SiGe.
- Defects in Hex-SiGe.
- First principles calculations of Hex-SiGe electronic properties.
- Modeling of Hex-SiGe structural and functional properties.
- Pressure-induced phase transitions: towards Hex-SiGe.
- Towards Hex-SiGe-based devices.
- III-Vs, II-VIs and related materials.

Recent advances, such as the demonstration of direct bandgap emission in hexagonal SiGe nanowires and improved modeling of phase stability, have significantly expanded the frontiers of this emerging material system. The workshop will provide a unique platform to exchange knowledge, discuss open challenges, and outline future directions for both fundamental research and technological applications.

2. Program

Monday 27th October		
08:30 - 09:00	Registration	
09:00 - 09:10	Presentation **Organizers**	
09:10 - 10:00	Keynote speaker **Friedhelm Bechstedt**	Chair **Emilio Scalise**
10:00 - 10:40	Invited speaker **Chris G. Van de Walle**	
10:40 - 11:00	**Christopher A. Broderick**	
11:00 -11:20	**Coffee Break**	
11:20 - 12:00	Invited speaker **Michele Re Fiorentin**	Chair **Silvana Botti**
12:00 - 12:20	**Esther van de Logt**	
12:20 – 12:40	**Madiha M. Makhdoom**	
12:40 – 14:40	**LUNCH POSTER SESSION**	
14:40 – 15:20	Invited speaker **Bianca Haberl**	Chair **Alexandre Courac**
15:20 – 16:00	Invited speaker **Kiran Mangalampalli**	
16:00 - 16:20	**Coffee Break**	
16:20 – 17:00	Invited speaker **Steffen Meder**	Chair **Erik Bakkers**
17:00 – 17:20	**Veronica Regazzoni**	
17:20 – 17:40	**Corentin Chatelet**	
18:45	**Social Dinner**	

Tuesday 28th October		
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09:40 - 10:00	**Ries Koolen**	
10:00 - 10:20	**Andrea Besana**	
10:20 - 10:40	**Kyriaki Samioti**	
10:40 - 11:00	**Perpetua W. Muchiri**	
11:00 - 11:20	**Coffee Break**	
11:20 - 12:00	Invited speaker **Jos E.M. Haverkort**	Chair **Laettitia Vincent**
12:00 - 12:20	**Riccardo Farina**	
12:20 - 12:40	**Denny Lamon**	
12:40 - 14:00	**LUNCH**	
14:00 - 14:40	Invited speaker **Anna Marzegalli**	Chair **Christopher A. Broderick**
14:40 - 15:00	**Frank Glas**	
15:00 - 15:20	**Fabrizio Rovaris**	
15:20 - 15:40	**Mette F. Schouten**	
15:40 - 16:00	**Hafssa Ameziane**	
16:00 – 16:20	**Twente conference announcement** **Coffee Break Closing Session**	

Monday 27th October

08:30-09:00	**Registration**
9:00-9:10	**Presentation**
09:10-10:00	**Friedhelm Bechstedt,** Friedrich-Schiller-Universitaet Jena **Light emission from hexagonal SiGe?**
10:00-10:40	**Chris G. Van de Walle,** University of California, Santa Barbara **First-principles theory of optical emission from hexagonal Ge**
10:40-11:00	**Christopher A. Broderick,** School of Physics, University College Cork **Electronic and optical properties of stacking faults in hexagonal germanium**
11:00-11:20	**COFFE BREAK**
11:20-12:00	**Michele Re Fiorentin,** Politecnico di Torino **First-principles study of optical properties of hexagonal Si and Ge nanowires**
12:00-12:20	**Esther van de Logt,** University of Twente **Electrical characterization of hexagonal silicon-germanium nanowires**
12:20-12:40	**Madiha M. Makhdoom,** University of Padova **Composition dependent bandgap and thermal conductivity in hexagonal SiGe alloys: a DFT approach**
12:40-14:40	**LUNCH AND POSTER SESSION**
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15:20-16:00	**Kiran Mangalampalli,** SRM University A. P. **Localized synthesis of mosaic hexagonal silicon via nanoindentation: reversible phase transformation and nanoscale electrical diagnostics**
16:00-16:20	**COFFE BREAK**
16:20-17:00	**Steffen Meder,** Walter Schottky Institut, Technical University of Munich **Integration of hexagonal SiGe into silicon photonic nanostructures**
17:00-17:20	**Veronica Regazzoni,** Università di Milano Bicocca **Electronic properties of perfect dislocations in germanium: a first-principles study**

17:20-17:40	**Corentin Chatelet,** C2N, CNRS, Université Paris-Saclay **Growth and characterization of hexagonal GaAs thin film on ZnS-4H**
18:45	**SOCIAL DINNER**

Tuesday 28th October

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09:40-10:00	**Ries Koolen,** Eindhoven university of technology **Progress in planar hex-Ge grown on metal sulfide substrates**
10:00-10:20	**Andrea Besana,** Department of Physics, Politecnico di Milano **Planar hexagonal germanium grown on cadmium sulfide substrate by low-energy plasma-enhanced chemical vapor deposition**
10:20-10:40	**Kyriaki Samioti,** Laboratoire de Physique des Solides, Université Paris-Saclay **Experimental study of the electronic band structure of hexagonal GaAs**
10:40-11:00	**Perpetua W. Muchiri,** Laboratoire de Physique des Solides, Université Paris-Saclay **Dopant interactions with I3-basal stacking faults in hexagonal silicon: first-principles insights into fundamental mechanisms**
11:00-11:20	**COFFE BREAK**
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12:40-14:00	**LUNCH**
14:00-14:40	**Anna Marzegalli,** Università di Milano Bicocca **Towards Hexagonal Germanium via Nanoindentation**
14:40-15:00	**Frank Glas,** C2N, CNRS, Université Paris-Saclay **The role of the contact angle in the hexagonal/cubic transition in semiconductor nanowires**
15:00-15:20	**Fabrizio Rovaris,** Università di Milano Bicocca **Origin and evolution of I3 defects in hexagonal silicon and germanium**
15:20-15:40	**Mette F. Schouten,** Eindhoven university of technology **Increased hexagonality in hex-SiGe core-shell nanowires**

15:40-16:00	**Hafssa Ameziane,** C2N, CNRS, Université Paris-Saclay **Growing SiGe nanowires with the hexagonal phase**
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Poster session

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P1	**Claudius S. A. Müller,** University of Twente **Realization of Ohmic Contacts on hexagonal SiGe Nanowires**
P2	**Anirban Das,** Institute of Physics, Budapest University of Technology and Economics **Hexagonal Germanium Nanowires as a Spin Qubit Platform**
P3	**Hadrien Le Petit,** Walter Schottky Institut, Technical University of Munich **Integration of Hex-SiGe into a NW-induced Photonic Crystal Cavity**
P4	**Dingshan Liu,** Walter Schottky Institut, Technical University of Munich **Exploring spin dynamic properties of direct-bandgap hex-SiGe for On-Chip silicon photonics applications**
P5	**Yetkin Pulcu,** University of Konstanz **Electronic and optical properties of hexagonal SiGe and GeSn alloys: a combined first-principles and k·p investigation**
P6	**Regis Andre,** Institut NEEL - CNRS **Pseudo-substrates, based on m-plane ZnS, for hexagonal SiGe growth**
P7	**Antonio M. Mio,** CNR-IMM Catania **TEM analysis of textured silicon polymorph crystals obtained via nanoindentation and annealing**
P8	**Fabrizio Rovaris,** Università di Milano Bicocca **Pressure-dependent kinetics of phase transitions in Si and Ge using machine learning interatomic potentials**
P9	**Órla N. McElhatton,** School of Physics, University College Cork **Empirical tight-binding Hamiltonian for cubic and hexagonal Ge: parametrisation from first-principles calculations**
P10	**Cedric Gonzales,** University of Basel **Chemical vapor deposition growth of Ge/Si-based nanowire heterostructures as hole spin qubit device platforms**
P11	**Marvin Marco Jansen,** Eindhoven university of technology **Silicon germanium interdiffusion in hexagonal SiGe heterostructures**
P12	**Sahar Gaddour,** Groupe d'Étude de la Matière Condensée (GEMaC) **Structural characterization of Cd1-xZnxS thin films grown on GaAs and on a- and m-plane wurtzite CdS substrates by metalorganic chemical vapor deposition for the synthesis of hexagonal Si_xGe_{1-x} layers**
P13	**Alexandre Courac,** IMPMC, CNRS, Sorbonne university **Crystallography of silicon element: stable and metastable crystalline forms**

3. Abstracts

Keynote speaker

Invited speakers

Contributed talks

Poster presentations

Talks

Light emission from hexagonal SiGe?

Friedhelm Bechstedt[1]

[1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

For decades a variety of approaches has been explored to obtain efficient light emission from group-IV semiconductors silicon (Si) and germanium (Ge), thereby to overcome the limitation due to the indirect gap of cubic (diamond) crystals. Recently, the collaboration of theoreticians, growers and spectroscopists have demonstrated that hexagonal (lonsdaleite, 2H) Ge-rich Si_xGe_{1-x} crystals are direct semiconductors with strong optical transitions explainable by band folding (Fig. 1) and wave-function mixing [1]. Even light emission from Ge-rich hexagonal quantum well (QW) structures could be observed [2].

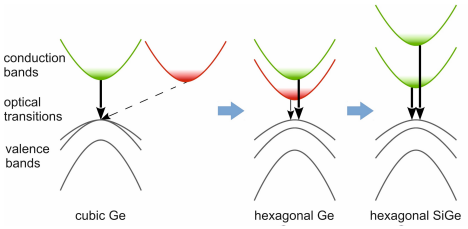

Fig.1. Optical transitions vs crystal structure and composition via band folding arguments.

We demonstrate that by controlling the composition, the emission IR wave length can be continuously tuned from 3.5 (Ge) to 1.8 ($Si_{0.35}Ge_{0.65}$) µm, corresponding to a direct-gap variation between 0.3 to 0.7 eV, thereby revealing excellent agreement between theoretical predictions for bulk alloys [3] and photoluminescence measurements of hexagonal SiGe shells grown on wurtzite-GaAs or -GaP nanowires [1]. The direct-indirect transition happens for about 45 % Si incorporation. The lowest-energy optical transition in hex-Ge is allowed for in-plane polarization [4]. The calculations predict increasing oscillator strength with lattice perturbation and chemical composition x (see Fig. 1) toward values as known from direct III-V semiconductors [5]. Still discrepancies between measurements and theoretical studies remain for 2H-Ge. Other polytypes, e.g. 4H-Ge, are found to be less applicable in optoelectronics.

Recently, QWs grown in [1-100] direction show light emission up to room temperature, whose frequency is tuned with the QW thickness [2]. The measured emission wave lengths and their thickness dependence well agree with theoretical predictions [6]. Band structure studies including the quasiparticle excitation aspect predict a type-I character of Ge-rich hexagonal SiGe QW structures with strain-dependent band offsets in the range of 0.06 – 0.26 eV resulting in a finite number of quantized levels and significantly varying optical transition strengths between conduction and valence subbands [7]. Mainly n=1 to n=1 subband transitions contribute. An interpretation of the confinement effects in terms of finite QW models is possible.

As a breakthrough light emission from Ge-rich hexagonal SiGe layers or QWs is not only predicted but also realized. It is shown that hexagonal SiGe embodies an ideal material system to combine electronic and optoelectronic functionalities on a single chip, opening the way toward integrated device concepts and information technologies.

[1] E.M.T. Fadaly et al., *Nature* **580**, 205 (2020)
[2] W.H.J. Wouters et al., *Nature Commun*. **15**, 5252 (2024)
[3] P. Borlido et al., *Phys. Rev. Mater.* **5**, 114604 (2021)
[4] C. Rödl et al., *Phys. Rev. Mater.* **3**, 034602 (2019)
[5] A. Belabbes et al., *Phys. Stat. Sol. RRL* **16**, 2100555 (2022)
[6] V.T. van Lange et al., *ACS Photonics* **11**, 4258 (2024)
[7] A. Belabbes et al. *Phys. Rev. B* **106**, 085303 (2022); ACS Appl. Mat. Int. (2025)

First-principles theory of optical emission from hexagonal Ge

Christopher A. Broderick[1,2,3], Xie Zhang[4], Mark E. Turiansky[1,5], and **Chris G. Van de Walle**[1]

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[2]School of Physics, University College Cork, Cork T12 YN60, Ireland.
[3]Tyndall National Institute, Lee Maltings, University College Cork, Cork T12 R5CP, Ireland.
[4]School of Materials Science and Engineering, Northwestern Polytechnical University, Xi'an 710072, China.
[5]US Naval Research Laboratory, 4555 Overlook Avenue SW, Washington, DC 20375, U.S.A.

The emergence of hexagonal Ge (2H-Ge) as a candidate direct-gap group-IV semiconductor for Si photonics mandates rigorous understanding of its optoelectronic properties. Theoretical predictions of a “pseudo-direct” band gap, characterized by weak oscillator strength, contrast with a claimed high radiative recombination coefficient B comparable to conventional (cubic) InAs. We present a rigorous theoretical analysis, based on first-principles calculations, of optical emission from 2H-Ge. We compute the radiative recombination coefficient B and quantify its dependence on temperature, carrier density and strain. For unstrained 2H-Ge, our calculated spontaneous emission spectra corroborate that measured photoluminescence corresponds to direct-gap emission, but with B being approximately three orders of magnitude lower than in InAs. We also confirm that ~ 2% [0001] uniaxial tension produces a pseudo-direct- to direct-gap transition which enhances B by up to three orders of magnitude.

We also discuss the potential to enhance the radiative recombination rate by forming polytype heterostructures, consisting of alternating cubic (3C) and hexagonal (2H) regions along the [111]/[0001] crystallographic axis. We confirm the presence of type-I band offsets at 2H/3C-Ge junctions, with electrons and holes confined in 2H-Ge. Quantum confinement allows to tune the emission wavelength within the application-rich 3–5 μm mid-infrared spectral range. We demonstrate that the optical matrix element can be increased by up to an order of magnitude in short-period 2H/3C superlattices. The presence of atypical miniband dispersion in such superlattices introduces a trade-off that must be engineered to optimize optical emission.

Electronic and optical properties of stacking faults in hexagonal germanium

Christopher A. Broderick[1,2,*], Mouad Bikerouin[3,*], Anna Marzegalli[3], Chris G. Van de Walle[4], and Emilio Scalise[3]

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[2]Tyndall National Institute, Lee Maltings, University College Cork, Cork T12 R5CP, Ireland
[3]Department of Materials Science, University of Milano-Bicocca, Via R. Cozzi 55, I-20125 Milano, Italy
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Direct-gap hexagonal (2H) Ge is most commonly realized by growing [0001]-oriented nanowires on a [111]-oriented cubic (3C) substrate [1]. The metastability of 2H-Ge has been observed to readily allow for defect formation via basal stacking faults (BSFs) in the (0001) plane [2]. Of these defects, the I3 BSF (a disruption of the twofold “AB” stacking sequence via a single “C” double layer) occurs frequently. Other BSFs [3], including intrinsic I1 and I2 defects (respectively consisting of one and two violations of twofold AB stacking), and extrinsic E defects (inclusion of an additional “C” double-layer), can potentially occur.

We perform a systematic analysis of the impact of BSFs on the optoelectronic properties of 2H-Ge, using first-principles (density functional theory) calculations [4]. Specifically, we quantify the impact of BSFs on the (i) electronic structure, (ii) interband optical matrix elements, and (iii) spontaneous emission.

The BSF electronic structure is interpreted via effective (zone unfolding) band structure calculations. Projecting the effective band structure (spectral function) onto atoms in pristine and faulted regions of BSF supercells allows to quantify carrier localization and its contribution to the perturbed band-edge states. We find that BSFs in 2H-Ge generally act as potential barriers, with the conduction and valence band edge states localizing outside of a given BSF. This suggests that BSFs in 2H-Ge are not expected to act as non-radiative (Shockley-Read-Hall) recombination centers. The calculated interband optical matrix elements and emission spectra demonstrate sensitivity to band hybridization. This band hybridization is induced by broken translational symmetry along [0001], a consequence of BSF formation, and makes the calculated properties sensitive to supercell size – i.e. to linear defect density along [0001]. For example, an I3 BSF can either decrease or increase the zone-center direct-gap optical matrix element, depending on defect density. Qualitative consequences of BSFs for device applications of 2H-Ge will be discussed.

[1] E.M.T. Fadaly et al., *Nature* **580**, 205 (2020)
[2] E.M.T. Fadaly et al., *Nano Lett.* **21**, 3619 (2021)
[3] C. Stampfl and C. G. Van de Walle, *Phys. Rev. B* **57**, R15052 (1998)
[4] C.A. Broderick, X. Zhang, M. E. Turiansky, and C. G. Van de Walle, arXiv:2412.08865 (2024)

*C.A.B. and M.B. contributed equally to this work.

First-Principles Study of Optical Properties of Hexagonal Si and Ge Nanowires

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I will discuss a first-principles investigation of the optical response of hexagonal-diamond (2H) Si and Ge nanowires, based on hybrid-functional electronic structure calculations combined with many-body perturbation theory (BSE) [1]. Optical absorption and electron energy loss (EELS) spectra were computed for both in-plane and out-of-plane polarizations and compared with high-resolution STEM-EELS measurements.

The simulated spectra reproduce the experimental features with remarkable accuracy, including the absorption onset in 2H-Si above 2.5 eV and a prominent peak at 3.7 eV, confirming the significantly reduced optical gap compared to cubic Si. For 2H-Ge, the calculations confirm the dipole-forbidden nature of the Γ-point transition, explaining the absence of low-energy absorption in the EELS spectra, while the strong ~2 eV peak observed in aloof-beam EELS is attributed to a thin 3C-Ge shell. Ongoing calculations of exciton radiative lifetimes aim to clarify which excitonic states contribute to light emission in 2H-Ge.

Overall, this study benchmarks ab initio predictions against nanoscale optical measurements and provides a coherent description of the optical response in 2H-Si and 2H-Ge.

[1] L.H.G. Tizei, M. Re Fiorentin et al., *Nano Lett.* **25**, 21, 8604–8611 (2025)

Electrical Characterization of Hexagonal Silicon-Germanium Nanowires

Esther van de Logt[1], Claudius Müller[1], Femke Witmans[1], Anouk Somhorst[1], Denny Lamon[2], Marvin Jansen[2], Erik Bakkers[2], Joost Ridderbos[1], and Floris Zwanenburg[1]

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[2]Eindhoven University of Technology, PO box 513, 5600MB, Eindhoven, The Netherlands.

Silicon and germanium, two of the most prevalent materials used in the semiconductor industry, are commonly used in their cubic (3C) crystal phase and therefore possess an indirect bandgap. Achieving a direct bandgap in these materials would open exciting new possibilities to combine conventional semiconductor techniques with photonics and to investigate novel spin-photon interfaces. The hexagonal (2H) crystal phase of Si/Ge alloys, known as hex-GeSi, has emerged as a promising material due to possessing a direct bandgap, in contrast to the cubic (3C) crystal phase [1-3].

Within the ONCHIPS and the Qumat consortium, we perform electrical transport measurements on hex-GeSi nanowires in order to investigate their fundamental transport properties and to eventually realize quantum dots (QDs). The nanowires are grown by a novel technique using molecular beam epitaxy and feature diameters down to 10nm [4, 5].

The extremely small diameters of these nanowires as well as the known properties of holes in Ge make this material platform an ideal candidate to investigate spin qubit physics [6-8].

Here, we present the fundamental transport properties of 2H-GeSi nanowires and the first results on the realization of electrostatically defined QDs. In the coming months, the nanowires will be placed on bottom gate arrays with a 70nm pitch to achieve even better QD control and eventually Pauli spin blockade in a double QD geometry.

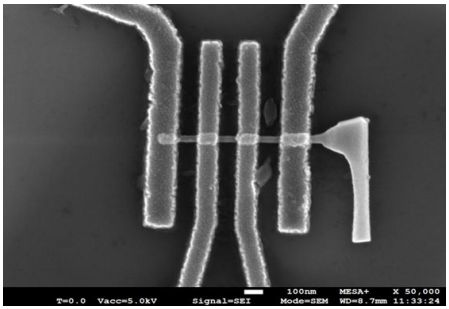

Fig. 1. SEM image of a hexagonal silicon germanium nanowire with titanium palladium contacts (10/80nm).

[1] C. Rödl et al., *Phys. Rev. Mater.* **3**, 034602 (2019)
[2] T. Kaewmaraya et al., *J. Phys. Chem. C* **121**,10, 5820–5828 (2017)
[3] E.M.T. Fadaly et al., *Nature* **580**, 205 (2020)
[4] A. Li et al., *Nanotechnology* **34**, 015601 (2022)
[5] D. Lamon et al., *Nano Lett.* **25**, 14, 5741–57462025 (2025)
[6] S. Conesa-Boj et al., *Nano Lett.* **17**, 4, 2259–2264 (2017)
[7] F. N. M. Froning et al., *Appl. Phys. Lett.* **113**, 073102 (2018)
[8] M. Brauns, et al., *Appl. Phys. Lett.* **109**, 143113 (2016)

Composition Dependent Bandgap and Thermal Conductivity in Hexagonal SiGe Alloys: A DFT Approach

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[1]Department of Materials Science, University of Rome "La Sapienza", Piazzale Aldo Moro 5, 00185 Rome, Italy
[2]National Institute of Nuclear Physics, Via Francesco Marzolo, 8, 35131 Padova PD

Hexagonal silicon-germanium ($Si_{1-x}Ge_x$) alloys have recently drawn attention due to their potential for advanced infrared photonics and efficient thermoelectric applications. In this study, we present a systematic theoretical investigation of their optoelectronic and thermal transport properties using first principles calculations performed with density functional theory (DFT) using Quantum ESPRESSO. Phonon thermal conductivity calculations were done using the Boltzmann transport equation.

Our results show that increasing Ge content leads to a nonlinear reduction in the direct bandgap from approximately 1.6 eV in pure hexagonal Si to about 1.0 eV in pure hexagonal Ge, shifting the absorption edge deeper into the infrared regime. Additionally, calculated exciton binding energies exhibit a significant increase around mid-range alloy compositions, suggesting enhanced optical activity. Thermal transport calculations show minimum in lattice thermal conductivity around x = 0.4 at room temperature due to increased alloy scattering effects.

These insights into the optoelectronic and thermal transport behaviors of hexagonal SiGe alloys provide valuable guidance for composition optimization, offers a potential high-performance infrared optoelectronic devices and thermoelectric materials.

Nucleation of hexagonal Si from bc8-Si on thermal annealing - Impact of sample volume and residual stresses on phase behavior

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[1]Neutron Scattering Division, Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA
[2]Department of Materials Physics, Research School of Physics, The Australian National University, Canberra, ACT 0200, Australia

The nucleation of hexagonal silicon (hex-Si) from the body-centered cubic bc8-Si phase upon thermal annealing to ~200°C was first reported over 60 years ago by Wentorf and Kasper [1]. This metastable phase has been difficult to characterize because it typically does not present as a well-formed crystal structure when made via annealing from bc8-Si. This has made the investigation of phase behaviors by diffraction methods or also by optical vibrational spectroscopy complex and confounding. Furthermore, the exact details of the pressure synthesis and resulting starting metastable Si (from which hex-Si is nucleated) also have critical influence.

Here, we investigate the annealing kinetics of the starting bc8 phases to hex-Si using nanovolumes synthesized through indentation loading, μm^3 volumes made in diamond cells, and an 80 mg large sample made in a Paris-Edinburgh press. While the nanovolumes of bc8-Si (and closely related rhombohedral r8-Si) made by indentation transform first into a phase with unknown structure, Si-XIII, recent work using a combination of Raman spectroscopy and electron diffraction established that eventually the entire nanovolume fully transforms to hex-Si [2]. Annealing under moderate pressures in a diamond cell probed with *in situ* synchrotron X-ray diffraction initially observed unidentified features upon annealing at ~3-4 GPa [3], yet more recent follow-up studies with varying hydrostaticity yield hex-Si directly at temperatures below 200°C. Finally, the annealing behavior of an 80 mg sample of bc8-Si was probed using time-resolved neutron spectroscopy, a technique less susceptible to issues with poor crystal nucleation. The material commenced to anneal directly to hex-Si at temperatures as low as 130°C. Collectively, these data illustrate an intriguing dependence on residual stresses and on material volumes and provide new insights into the phase behavior and formation mechanism of bulk hex-Si from pressure-derived precursor phases.

This research used resources at the ARCS Spectrometer and the SNAP Diffractometer of the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory under Proposal No. 34994. This research also used resources at HPCAT, Sector 16, of the Advanced Photon Source a DOE Office of Science User Facility operated by Argonne National Laboratory under Proposals No. 38217 and 42166.

[1] R.H. Wentorf Jr., and J.S. Kasper, *Science* **139**, 338 (1963)
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Localized Synthesis of Mosaic Hexagonal Silicon via Nanoindentation: Reversible Phase Transformation and Nanoscale Electrical Diagnostics

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Hexagonal diamond silicon (hd-Si, or hex-Si) has long been recognized for its extraordinary optoelectronic potential, including the prospect of a direct and tunable bandgap superior to conventional diamond-cubic silicon (dc-Si). Realizing stable, scalable forms of hd-Si remains a technological hurdle due to its metastable nature and complex phase relationships with other high-pressure silicon allotropes. Here, we demonstrate the direct local synthesis of large-area, micron-scale textured domains of hd-Si within single-crystal dc-Si wafers by combining instrumented spherical nanoindentation with controlled vacuum annealing (250–1000 °C).

Comprehensive characterization by Raman spectroscopy, high-resolution transmission electron microscopy (HRTEM), and electron diffraction reveals that annealing indented regions at intermediate temperatures (350–700 °C) produces highly textured, mosaic microstructures composed of multiple hexagonal polytypes—specifically 2H, 4H, and 6H stacking sequences. These mosaic domains are confined laterally (2–3 μm) and horizontally (~6 μm) within an otherwise untransformed Si matrix, offering precise spatial selectivity compatible with device miniaturization.

The mechanical and electronic behavior of these metastable phases was probed in situ using nanoelectrical contact resistance (nanoECR) measurements during Berkovich nanoindentation. Strikingly, hd-Si and annealed nanocrystalline dc-Si exhibited reversible pressure-driven phase transitions: under mechanical loading, both phases transformed into the metallic β-Sn phase, reverting to a mixture of R8 and BC8 polymorphs upon unloading. This transformation pathway, previously only predicted by theory, is now confirmed experimentally through correlated Raman, TEM, and in situ nanoECR measurements. Subsequent high-temperature annealing (>900 °C) facilitates further reversion to nanocrystalline dc-Si, with residual traces of hexagonal phases, highlighting the thermally driven reversibility and instability of hd-Si under ambient conditions.

This work not only provides microscopic and electrical evidence for reversible phase transformations among high-pressure Si allotropes but also establishes nanoindentation-coupled annealing as a powerful, scalable, lithography-free strategy for mosaic hexagonal Si generation. The formation of mixed hexagonal polytypes (rather than pure 2H, 4H, or 6H) is attributed to the complex interplay of stacking faults, local strain fields, and kinetic constraints during transformation, and ongoing research seeks to selectively stabilize the 2H polytype—predicted to possess a direct bandgap via its simple ABAB stacking—through strategic stress modulation, and annealing. Such advances are poised to unlock CMOS-compatible direct-bandgap Si materials, potentially revolutionizing silicon photonics and energy conversion technologies.

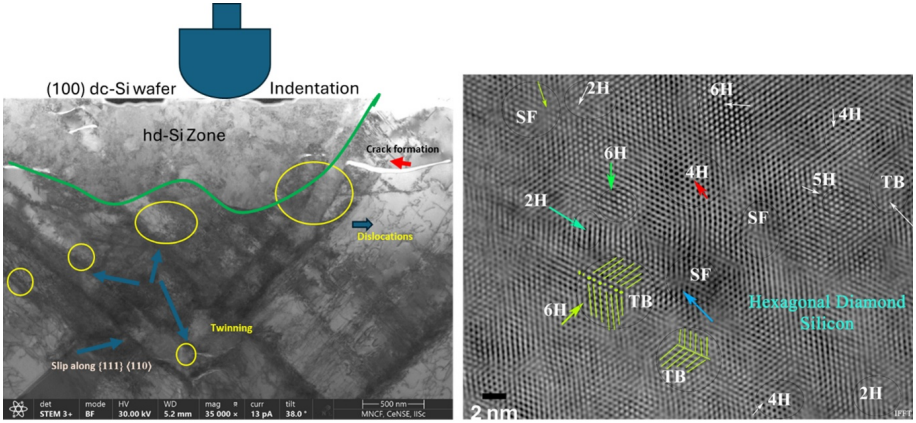

Fig. 1. Cross-sectional SEM and TEM images show primary slip along {111} planes, possible mechanical twinning, shear band formation, crack generation, dislocations, and sharp phase boundaries beneath the indented surface when indented along [100] on (100) dc-silicon surface. High-resolution TEM image of the 500°C annealed sample revealing stacking faults, twin boundaries, and hexagonal silicon polytypes (2H, 4H, 6H). These defects influence phase stability and transformation pathways, highlighting the complex interplay between residual strain, crystallographic defects, and polytype formation in metastable silicon phases.

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Integration of hexagonal SiGe into silicon photonic nanostructures

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Cubic silicon (Si) is an indirect bandgap semiconductor and is therefore known for being an inefficient light emitter. In contrast, hexagonal SiGe (hex-SiGe) has been shown to exhibit a direct bandgap for a Ge content exceeding 67%. Since Si and Ge naturally crystallize in the cubic phase, Hex-SiGe is synthesized as a shell around a wurtzite (WZ) GaAs NW core using the crystal transfer method. By varying the Ge content, the emission wavelength can be tuned across a broad spectral range from 1.8 to 3.4 µm [1]. Taking steps towards realizing a hex-SiGe laser, individual NWs lying on an AlN substrate have been investigated and were shown to exhibit amplified spontaneous emission. Hakki-Paoli analysis indicates that reflection losses of the Fabry-Perot resonator significantly contribute to overall cavity losses with geometrical Q-factors around 60. This suggest that conventional mirror-based feedback is insufficient to exceed threshold for lasing [2].

In this talk, I will discuss our recent work aiming at enhancing optical feedback by inserting single hex-SiGe nanowires into silicon photonic crystals to form self-localized photonic modes [3]. Hereby, we use PDMS/PC transfer printing approaches to precisely manipulate the nanowire into a slot defect. We explore the self-localized resonant modes emerging from a comparable dielectrically loaded slot waveguide cavity through introducing a Si segment in top-down fabrication (Figs 1a and 1b). Cross-polarized reflectance spectroscopy provides valuable insights into optimizing photonic crystal cavities for mid-infrared wavelengths. For our application, the resonance energy can be tuned within the range of 0.465 eV to 0.61 eV by adjusting lattice constant and hole radius to cover the full emission range of hex-$Si_{0.2}Ge_{0.8}$. Our findings indicate that the optical modes are predominantly determined by the photonic crystal geometry rather than the segment geometry, as evidenced by the limited sensitivity to changes in segment length and position (Fig. 1c). For longer segments, we observed higher order PhC cavity modes and studied their spatial overlap with the segment (Fig. 1d). Results obtained using hex- SiGe will be contrasted with similar devices realized using InAs and GaAsSb NWs.

Work performed by J. Zöllner and S. Meder, with assistance of H. Petit-Delacourt and D. Liu at TUM using materials grown by the group of Erik Bakkers at TU/Eindhoven.

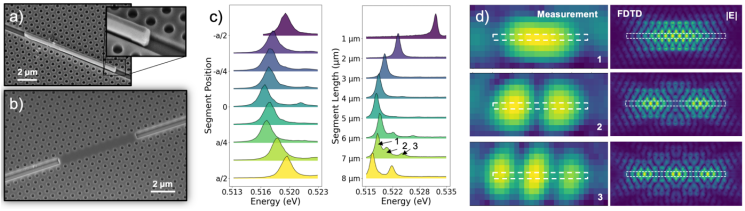

Fig 1. a) SEM image of a hex-SiGe NW transferred into the slot waveguide cavity. b) Top-down etched Si segment allowing systematic studies of resonant modes. c) spectra from cross-polarized reflectance spectroscopy. d) Measurements of spatially resolved mode profiles of a 7 µm long segment and FDTD simulations.

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Electronic Properties of Perfect Dislocations in Germanium: A First-Principles Study

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The epitaxial growth of Ge on Si substrates involves the accumulation of internal strain due to the 4% lattice mismatch between the two materials. When plastic relaxation occurs, dislocations in the Ge sample are formed, consisting in Misfit Dislocations (MDs) connected to their Threading Dislocations (TDs) arms. While this represents a unavoidable detrimental aspect in the technique, no conclusive quantitative results on the effective impact of perfect MDs and TDs dislocations on the electronic properties of bulk Ge can be found in the literature.

In this study we evaluated the electronic structures via ab initio calculation using the Vienna Ab initio Simulation Package (VASP) [2] and we studied the electronic properties of Ge by exploiting the meta-GGA approach of Tran and Blaha, based on the modified Becke–Johnson (mBJ) exchange potential [3], known to correctly predict the bulk Ge band structure.

To predict the defect energy levels induced in bulk Ge band structure we unfolded the band structure into the Brillouin Zone of the primitive cell of Ge and projected the band structure on the dislocation atoms.

From the unfolding and the projection on the bulk atoms of the band structure of the defected systems it is also possible to identify the effect on the electronic structure due to the spurious strain field associated with a dislocation in a finite supercell. Direct inspection of data reported in Fig.1 reveals a good correspondence between the band structure of the bulk present in our supercells and the band structure of a primitive cell. By projecting on the dislocation core atoms, the effect induced by the dislocations themselves can be identified, and the dislocations dispersive band can be found.

This work establishes a basis for future studies on the interplay between dislocations and point defects in Ge, extending the understanding of their impact on the electronic and optical properties of Ge.

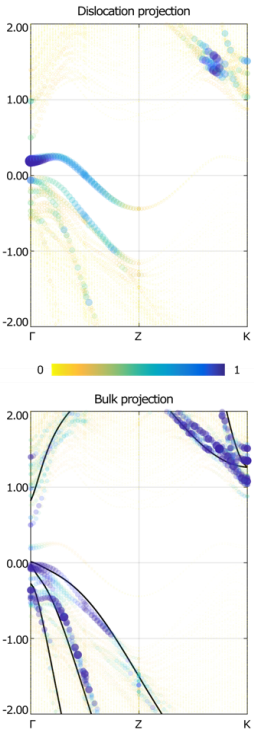

Fig.1. Unfolded band structure of the S3 shuffle 60° dislocation, projected on dislocation atoms (top panel) and on the bulk atoms. When the band is projected on the bulk atoms (bottom), the primitive cell Ge band structure is also shown by a solid black line.

F.M. gladly acknowledges financial support by the European Union – NextGenerationEU – Investment 1.1, M4C2 - Project Title “NANOSEES” n. P2022YM8J3 – CUP D53D23018720001 - Grant Assignment Decree No. 1389 adopted on 01st September 2023 by the Italian Ministry of Ministry of University and Research (MUR)

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Growth and Characterization of hexagonal GaAs thin film on ZnS-4H

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Phase engineering has emerged as a powerful approach to tune the electronic band structure of semiconductors offering novel pathways for advanced technological devices [1]. A notable example is GaAs in the hexagonal 2H phase, demonstrated in nanowires, which exhibits a slightly modified band structure compared to its stable cubic counterpart according to calculations. However, there is not yet consensus on the band gap of GaAs-WZ. Overall, NWs make difficult the investigation of basics properties: size, morphology, strain and surface states inherent to surface/volume ratio may explain the large disparity of band gap and band offset measurements [2]. And the calculations either remain a highly controversial story. Beyond nanowires, the synthesis of thin films of metastable GaAs polytypes is a critical step toward scalable integration and the realization of direct-band-gap group-IV/III–V platforms.

In this work, we focus on the epitaxy of metastable hexagonal GaAs polytype by metal-organic chemical vapor deposition (MOCVD). The methodology relies on the use of a stabilized hexagonal substrate of ZnS-4H with the specific m-plane surface. Under specific growth conditions, GaAs can be stabilized in the 4H form, minimizing stacking faults and other crystallographic defects critical for high-quality films.

A comprehensive multi-technique characterization strategy was employed to assess structural and optical quality: X-ray diffraction (XRD) for crystal structure and phase purity, Raman spectroscopy for phonon modes, second-harmonic generation (SHG) to confirm non-centrosymmetric symmetry, photoluminescence (PL) and cathodoluminescence (CL) to probe optical response, light scattering for structural coherence, and angle-resolved photoemission spectroscopy (ARPES) to directly investigate the electronic band structure. These results demonstrate that controlled phase engineering on pseudo-substrates enables scalable synthesis of hexagonal GaAs thin films, opening pathways for next-generation photonic, thermoelectric, and quantum devices based on metastable III–V polytypes.

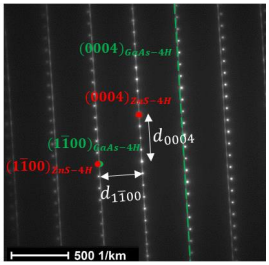

Fig. 1. Diffraction pattern recorded at the GaAs/ZnS interface showing the epitaxial alignment of GaAs with ZnS.

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Growth of hexagonal Ge on GaAs nanowires by molecular beam epitaxy

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Hexagonal group-IV semiconductors are attracting increasing attention as they offer electronic and optical properties distinct from their cubic counterparts, with potential applications in nanophotonics and quantum technologies [1]. Here, we present recent progress on the molecular beam epitaxy (MBE) growth of hexagonal germanium (Ge) on GaAs nanowire templates [2]. Careful control of growth parameters enables the stabilization of the metastable hexagonal phase, as confirmed by structural characterization.

The surface chemistry of the as-grown materials is investigated by X-ray photoelectron spectroscopy (XPS), revealing different As contamination pathways. Preliminary angle-resolved photoemission spectroscopy (ARPES) provides direct insight into the electronic band structure. Finally, we show recent advances in the fabrication of tailored structures achieved through selective chemical etching aimed at enhancing light matter interaction.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 801512. This work was supported by the LABEX iMUST of the University of Lyon (ANR-10-LABX-0064), created within the program « Investissements d'Avenir » set up by the french government and managed by the French National Research Agency (ANR).

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Progress in planar hex-Ge grown on metal sulfide substrates

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Experimental realization of hexagonal phase SiGe (hex-SiGe) has been attempted using a variety of techniques, ranging from core-shell nanowires to strain based transformation of nanofins [1,2]. Whilst these techniques have successfully realized hex-SiGe, the total volume remains limited, hindering both scalability for future devices and the breadth of available experimental techniques that can effectively assess its properties.

Hence, we aim to scale up the realized hex-SiGe volume by performing epitaxial growth on planar substrates. This approach not only offers a large effective area but also benefits from high reproducibility and process control

A requirement for growing hexagonal phase germanium is a single crystalline substrate that acts as an epitaxial template for the germanium. Cadmium Sulfide (CdS) substrates, which naturally crystallize in the hexagonal phase, have emerged as the most suitable candidate. CdS has a lattice mismatch of approximately 3% with hex-Ge and is commercially available in various substrate orientations. To overcome the 3% mismatch and virtually reduce it to 0%, we have successfully grown high quality $Cd_{0.65}Zn_{0.35}S$ buffer layers by elemental source MBE growth.

In this work we discuss the growth of hex-Ge layers on $Cd_{0.65}Zn_{0.35}S$ (10-10) & (11-20) virtual substrates via MBE. Various parameters such as growth temperature and Ge deposition rate have been probed. The structural characteristics of the Ge layer have been investigated by HRXRD and STEM analysis. Structural analysis has been correlated with macro photoluminescence measurements. These findings enable us to better understand the complex mechanisms occurring in heteroepitaxial growth of Ge on $Cd_{0.65}Zn_{0.35}S$ with the future aim of creating high quality hex-SiGe layers.

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Planar Hexagonal Germanium Grown on Cadmium Sulfide Substrate by Low-Energy Plasma-Enhanced Chemical Vapor Deposition

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Germanium (Ge) is a material of significant interest in the field of semiconductor technology due to its electronic and optical properties. The scientific community has recently intensified research efforts to obtain hexagonal Ge-2H which has been shown to exhibit a direct bandgap. The formation of Ge-2H has thus far been confined to nanodomains obtained mainly via core/shell nanowires [1]. This approach inherently restricts the active volume, thereby hindering fundamental property investigations and device fabrication. To overcome this constraint, it is therefore essential to synthesize high-quality planar Ge-2H crystals.

The main objective of this work is to grow Ge-2H layers on wurtzite bulk substrates with m-plane orientation. As bulk gallium arsenide does not exist in the wurtzite phase, hexagonal cadmium sulfide (CdS-2H) substrate was selected as an alternative hexagonal template, due to the closely matched lattice parameters with Ge. The Ge deposition was performed by Low Energy Plasma Enhanced CVD at low temperature (low-T) (200 – 300°C) in order to prevent Cd desorption from the substrate, which would lead to a substoichiometric surface and possibly result in the loss of the substrate's template effect on germanium growth. Prior to the low-T growths on CdS substrates, a preliminary study on low-T epitaxy on silicon substrates was conducted, obtaining crystalline thin Ge epilayers even at ultra-low-T (200°C).

The Ge/CdS samples were structurally characterized by HR-XRD, SEM-EDX, STEM, and Raman spectroscopy. In the first growth at 300°C, the resulting film displayed dendritic structures, approximately 40 nm thick, with observable Ge intermixing with CdS, as shown in Fig. 1a. This outcome is likely due to the excessive growth temperature. In the second growth, the temperature was reduced to 200°C, leading to the formation of an amorphous but compact Ge layer about 50 nm thick (as depicted in Fig. 1b). For the third growth, the temperature was increased to 250°C while the Ge layer thickness was limited to just 10 nm, specifically to rule out the possibility that excessive elastic energy from lattice mismatch caused the amorphization observed previously. Fig. 1c shows Raman spectra of the 10 nm-thick Ge/CdS sample, performed with rotating sample and fixed polarizer. In the configuration x(y,y)x, according to Porto notation and corresponding to 90° in the image, it is possible to detect the transverse optical E_{2g} mode of Ge-2H (at ~287 cm^{-1} [2]), whose intensity decreases until it disappears, moving towards the configuration x(z,z)x configuration (0° in the image). Further investigations, including PL measurements, will be performed as soon as possible to possibly confirm the successful planar Ge-2H growth.

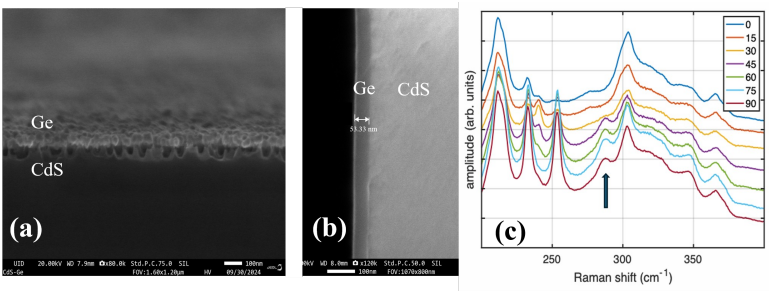

Fig. 1. Cross-section view SEM images of the first (at 300°C (a)) and second (at 200°C (b)) growths. (c) Raman spectra of the 10 nm-thick Ge/CdS sample (grown at 250°C), acquired in different configurations (x(y,y)x and x(z,z)x correspond to 90° and 0°, respectively).

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Experimental study of the electronic band structure of hexagonal GaAs

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Compound III-V semiconductors typically crystallize in the zinc blende structure, but can also, adopt the hexagonal wurtzite structure. This happens under specific growth conditions, as demonstrated for GaAs nanowires and other systems. The control of structural degrees of freedom provides a powerful means to tailor their optoelectronic properties, such as their bandgap size and carrier dynamics, their excitonic behavior, or even induce direct bandgaps, as observed in GaP and AlP which are indirect in their zinc blende phase. This phase engineering is very promising for the implementation of novel devices such as light-emitting diodes and solar cells. Furthermore, the control of hexagonal-phase semiconductors may as well facilitate their integration with other compounds in devices based on junctions and heterostructures. To this end, the experimental determination of the electronic band structure of the novel phases is of paramount importance.

Here, we present the first Angle Resolved Photoemission Spectroscopy (ARPES) measurements on hexagonal 4H-GaAs thin films grown on 4H-ZnS substrate. Our data reveal the n-nature of the thin films, with the valence band maximum located at Γ, around 1.5 eV below the Fermi level. Additionally, constant energy cuts display a hexagonally symmetric Fermi surface, directly reflecting the underlying lattice symmetry. These first results demonstrate the feasability of using ARPES to directly probe the band structure in this newly explored structural phase and lay the groundwork for deeper studies of the electronic properties of hexagonal GaAs, a crucial step for assessing its potential in future optoelectronic and quantum devices.

Dopant interactions with I_3-basal stacking faults in hexagonal silicon: first-principles insights into fundamental mechanisms

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Group IV semiconductors in the hexagonal phase have attracted considerable interest due to their unique electronic and optical properties, which differ significantly from their cubic counterparts [1]. A prominent structural feature of these materials is the presence of I3-basal stacking faults (BSFs) [2], which influence carrier dynamics and defect interactions. While the effects of point defects on the electronic properties of these materials are well understood [3-5], the interactions between these defects and extended structures such as BSFs remain largely unexplored.

In this work, we employ first-principles calculations based on density functional theory (DFT), using the SIESTA code, to investigate the behavior of acceptor and donor dopants in hexagonal silicon with BSFs [6]. Our results reveal distinct behaviors for the two types of dopants. Acceptor dopants tend to migrate away from the stacking fault, as their interaction with the planar defect reduces their stability [6]. On the other hand, donor dopants exhibit a lesser tendency to migrate, indicating that local strain distortions have a weaker effect on their incorporation. In both cases, dopant displacement depends on how well the impurity fits within the lattice and the nature of the electronic states involved [6].

These findings provide essential insights into the factors governing the stability and distribution of dopants in the presence of extended defects, offering valuable implications for the design and optimization of electronic devices.

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Optical properties of hex-SiGe

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Silicon germanium (SiGe) alloys are mainstream in electronics, but due to their indirect bandgap, they are not capable to emit light. In the hexagonal (hex) crystal structure, SiGe becomes a direct bandgap semiconductor [1] with a tunable bandgap between 3.4 μm for hex-Ge down to approximately 1.5 μm for hex-SiGe.

I will review the optical properties of hex-SiGe, which show a subnanosecond radiative recombination lifetime, a radiative efficiency comparable to a III/V semiconductor, and a low surface recombination velocity. Moreover, the hex-Ge/SiGe heterostructure shows type I band alignment, which allows to observe quantum confinement in hex-$Si_{1-x}Ge_x$/$Si_{1-y}Ge_y$ quantum wells [2] and which is promising for silicon compatible quantum well lasers and quantum dot single photon emitters. We finally observe stimulated emission from hex-SiGe nanowires. Most importantly, a Hakki-Paoli analysis of the stimulated emission properties reveals a material optical gain of >500 cm^{-1} [3], which is sufficient for lasing.

Despite these promising material properties, we still observe a large discrepancy with theoretical predictions. For the hex-SiGe alloys, the radiative efficiency might be high in the experiments due to the breaking of translational symmetry by alloy broadening. We can only speculate about the radiative lifetime of 2.1 ns and the oscillator strength of 10.5 in hex-Ge [4]. The properties of hex-Ge are again comparable to a III/V semiconductor, despite the fact that alloy broadening is absent here.

I like to acknowledge the European Union's Horizon 2020 research and innovation program with grant agreement number 964191, Opto Silicon, and the Dutch Organization for Scientific Research (NWO) Grants No. 024.002.033, 739.017.002, and OCENW.M.21.052.

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[4] V.T. van Lange et al., *ACS Photonics* **11**, 4258 (2024)

Heat Management in Hex-SiGe Nanowires for Silicon-Compatible Lasers

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Hexagonal silicon-germanium (hex-SiGe) alloys have emerged as promising direct-bandgap emitters, with stimulated emission recently reported in hex-SiGe nanowires (NWs) [1,2].

However, achieving stable lasing in hex-SiGe NWs remains challenging. The primary limitation is insufficient heat dissipation during optical excitation due to poor thermal coupling with the substrate, caused by the NW's rough side surface (Fig. 1a).

This work demonstrates how thin hexagonal boron nitride (hBN) flakes can improve heat dissipation from hex-SiGe NWs. We implement thin hBN flakes as thermal interface layers covering the nanowires (Fig. 1b), coupling them with a gold heat sink. Samples were characterized using micro-photoluminescence spectroscopy on individual nanowires (Fig. 1c-e), from which operating temperatures were extracted [3]. Comparison between NWs directly on substrate and those covered by hBN flakes reveals that improved thermal contact reduces operating temperatures by up to 500 K during optical excitation (Fig. 1f).

We conclude that interfacing nanowires with gold heat sinks via hBN flakes significantly enhances heat dissipation, particularly when thin flakes conform to the sidewalls. This improved thermal management enables higher excitation fluences than previously possible, bringing stable nanowire lasers closer to reality and removing the primary barrier to achieving silicon-integrated laser sources.

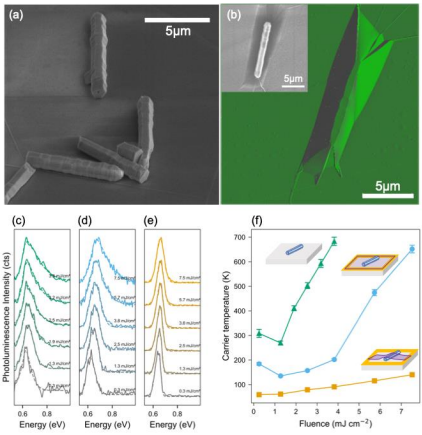

Fig. 1. (a) SEM picture of hex-SiGe NWs on AlN substrate; (b) AFM image of a nanowire under an hBN flake; inset shows the corresponding SEM image. (c-e) PL spectra as a function of excitation fluence for a NW in three configurations: on the AlN substrate (c), on top of a hBN flake (b), and covered (c); (f) extracted carrier temperature for the three configurations.

[1] E.M.T. Fadaly et al., *Nature* **580**, 205 (2020)
[2] M.A.J.van Tilburg et al., *Commun Physics* **7**, 328 (2024)
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Hexagonal SiGe Quantum Structures Realized in Nanowires

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The growth of axial heterostructures in nanowires has emerged as a powerful technique for fabricating advanced devices with broad technological impact. For example, III–V semiconductors have enabled the development of integrated photonic systems [1], memory devices [2], and quantum technologies [3]. In these regards, has recently emerged the possibility of fabricating light emitting quantum materials using SiGe alloys [4], key compound of semiconductor industry. Until now, however, hexagonal SiGe (hex-SiGe) quantum structures have only been realized in the form of two-dimensional quantum wells. In this work, we expand the scope of quantum heterostructures by showing the fabrication of both quantum wires and quantum dots in hex-SiGe. We demonstrate for the first time the fabrication of one-dimensional and zero-dimensional hexagonal SiGe heterostructures using an axial trunk–branch nanowire approach [5]. By precisely adjusting the precursor ratios during growth, we achieved accurate control over the Ge composition in each segment. The resulting structures exhibit sharp and symmetric interfaces of approximately 15 nm, along with excellent tunability of both diameter and length, key parameters for tailoring quantum confinement effects. This level of structural and compositional control opens up exciting opportunities for engineering quantum devices based on SiGe nanostructures.

This breakthrough completes the full dimensional suite of quantum confinement in this material system, opening exciting new opportunities for quantum and photonic device architectures expanding the frontiers of quantum silicon technology.

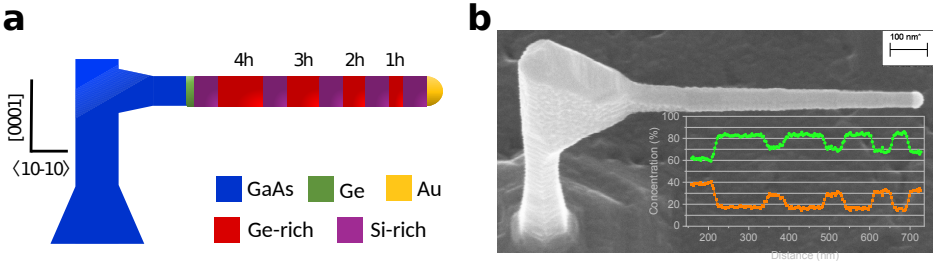

Fig. 1. Hexagonal SiGe heterostructures realized with trunk-branch growth approach. a) schematic illustration of Ge-rich segments of varying lengths embedded within Si-rich barriers. b) SEM image of a heterostructure branched nanowire and Energy-dispersive X-ray spectroscopy axial line-scan.

[1] Koval et. al., *Nanomaterials*, ***10,*** 11 (2020)
[2] Thelander et. al., *Nano Lett.*, *5*, 4 635-638 (2005)
[3] Thelander et. al., *Appl. Phys. Lett.*, ***83,*** 10 2052–2054 (2003)
[4] Peeters et. al., *Nat. Commun.*, ***15,*** *1* (2024)
[5] Lamon et. al., *Nano Lett.*, **25**, 14 5741–5746 (2025)

Towards Hexagonal Germanium via Nanoindentation

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Hexagonal germanium (hd-Ge) is typically realized through the template effect of a wurtzite structured core in core/shell nanowires [1]. In this work, we explore an alternative route based on nanoindentation, aiming to induce pressure-driven phase transitions to reach the metastable hexagonal phase.

We investigate phase transitions not only in germanium but also in silicon, with the goal of enabling subsequent deposition of Ge (or SiGe) on top of transformed regions. Here, we present a comprehensive theoretical and experimental study of micrometer-sized, textured hexagonal silicon (hd-Si) crystals formed via spherical nanoindentation followed by thermal annealing. Advanced characterization techniques, such as polarized Raman spectroscopy, high-resolution transmission electron microscopy (TEM), and electron energy-loss spectroscopy (EELS), reveal the formation of nanometer-sized grains with slight misorientation, arranged into larger coherent domains.

First-principles calculations and molecular dynamics simulations provide insight into the mechanisms of pressure-induced phase transformation, highlighting the critical role of both elastic and plastic deformation in stabilizing the hd-Si phase [2].

We also present first results on germanium, demonstrating the feasibility of the approach. Regions of hd-Ge were successfully obtained using sharp nanoindentation and unambiguously identified by polarized Raman spectroscopy and TEM diffraction. The indentation was carried out at low temperatures (between -30 °C and 10 °C), which effectively suppressed the widespread nucleation of extended defects, typically an alternative pathway to phase transformation under pressure.

Finally, we present Nudged Elastic Band (NEB) calculations indicating that germanium exhibits lower energy barriers for phase transformation upon unloading compared to silicon, which explains why no annealing step is required to stabilize hd-Ge in our approach.

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The role of the contact angle in the hexagonal/cubic transition in semiconductor nanowires

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Our understanding of the formation of the hexagonal structure during the vapor-liquid-solid (VLS) growth of nanowires (NWs) is largely based on two models and *in situ* transmission electron microscopy (TEM) experiments. The models apply to both elementary and compound semiconductors, although it is only in the latter case that the hexagonal structure, namely wurtzite (WZ), is frequently obtained and that its formation can be investigated *in situ*. We thus consider specifically III-V compounds.

The first model states that the position of the 2D nucleus that triggers the growth of each monolayer (ML) at the NW/liquid interface, determines the ML type, and that WZ may form if its nucleation barrier is lower than that of the cubic zinc blende (ZB) phase [1]. This requires that (1a) nucleation occurs at the triple phase line (TPL) bordering the interface, (1b) the energy of the lateral nucleus facet (or step) in contact with the vapor is lower for WZ than for ZB, (1c) liquid supersaturation is high enough. Condition (1a) has now been confirmed by *in situ* TEM [2,3] and (1b) is supported by *ab initio* calculations [4,5]. We shall thus focus on condition (1c).

The second model is based on other *in situ* TEM results showing that, in a given NW, the WZ/ZB transitions usually correlate with changes of the NW/liquid interface morphology between planar and "truncated", occurring at critical values of the droplet contact angle β, with WZ only present at intermediate β, along with a planar interface [6,7]. The model explains how β determines interface morphology, but does not address WZ/ZB selection, since it considers neither nucleation nor growth. However, putting together the two models, it may be inferred that WZ growth is inhibited if the TPL vanishes, as is the case if a truncation forms all around the NW. But this is probably usually not the case, and other explanations are being explored.

The droplet contact angle β plays a key role in both models, but there is no obvious reason for the critical angles for the structural and morphological transitions predicted by the first and second models, respectively, to be the same. Here, we focus on the WZ/ZB transition that occurs upon increasing contact angle well above $\beta=\pi/2$. We show that the contact angle at which WZ nucleation becomes favorable depends on the difference of chemical potential $\Delta\mu$ between liquid and solid at nucleation (and, more precisely, on the ratio between $\Delta\mu$ and the difference of cohesive energies between the two phases), with a maximum angle obtained at large $\Delta\mu$. In light of these calculations, and based on published data and recent modeling [8,9], we discuss the interaction between nucleation and truncation formation and what could be the reason for the correlation between the two.

[1] F. Glas, et al., *Phys. Rev. Lett.* **99**, 146101 (2007).
[2] J.C. Harmand, et al., *Phys. Rev. Lett.* **121**, 166101 (2018).
[3] M. Marnauza, et al., *Nanoscale Horiz.* **8**, 291 (2023).
[4] R. Magri, et al., *Phys. Status Solidi C* **7**, 374 (2010).
[5] V. Pankoke, et al., *Phys. Rev. B* **84**, 075455 (2011).
[6] D. Jacobsson, et al., *Nature* **531**, 317 (2016).
[7] F. Panciera, et al., *Nano Lett.* **20**, 1669 (2020).
[8] F. Glas, *Phys. Rev. Mater.* **8,** 043401 (2024).
[9] F. Glas, in preparation (2025).

Origin and Evolution of I3 defects in Hexagonal Silicon and Germanium

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Recently, hexagonal diamond (2H) SiGe has been synthesized by exploiting core/shell nanowires [1] and demonstrating the direct electronic bandgap for the Ge-rich 2H-SiGe shells [2]. However, due to the metastability of the 2H crystal phase, the inclusion of the most stable diamond cubic phase via defects appearing during the growth is easily understandable. Of particular importance is the I3 defect, very often present in the 2H-SiGe shell and has been analyzed in recent works [3], but questions about its origin and possible evolution after the shell growth are still open.

Here, we propose a general atomistic mechanism, supported by *ab initio* Density Functional Theory (DFT) calculations and Machine Learning (ML)-based Molecular Dynamics (MD) simulations, describing the formation of the I3 defect in different configurations, including the triangular and non-triangular shapes for the extended defects. In particular, we link its formation to the surface reconstruction during the growth, thus identifying its formation mechanism with a line-like origin, explaining all experimental evidence [4].

Furthermore, we propose a model for the atomistic evolution of such I3 defects based on Nudged Elastic Band Calculations. We evaluated the kinetic barriers for the kink formation and migration in silicon by exploiting an established ML interatomic potential [5], enabling an estimate of the total transition rate for the defect propagation. Preliminary results have also been obtained for germanium [6], highlighting the higher mobility of such defects in germanium shells with respect to the silicon case. These findings may suggest a procedure to minimize the extension of I3 defects by playing with alloying composition and growth conditions.

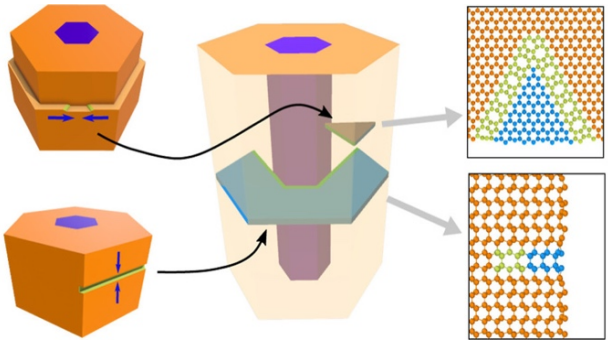

Fig. 1. Sketch of different shape configurations of I3 defects linked to their possible origin as surface reconstruction during the growth of the shell (left) and their atomistic view (right).

[1] H. Hauge et al., *Nano Lett.* **15** 5855-5860 (2015)
H. Hauge et al., *Nano Lett.* **17**, 85-90 (2017)
[2] E.M.T. Fadaly et al., *Nature* **580**, 205 (2020)
[3] E. Fadaly et al., *Nano Lett.* **21** 3619-3625 (2021)
L. Vincent et al., *Adv. Mater. Int.* **9**, 2102340 (2022)
[4] F. Rovaris et al. *ACS Appl. Nano Mater.* **7** 9396−9402 (2024)
[5] J. Dellevoet et al., in preparation (2025)
[6] A. Fantasia et al., *J. Chem. Phys.* **161**, 014110 (2024)

Increased hexagonality in hex-SiGe core-shell nanowires

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To mitigate the ever-increasing energy demands of data storage, significant research effort is being devoted to achieving light emission from group IV semiconductors. Recently, hexagonal silicon germanium (hex-SiGe) has emerged as a promising candidate for a silicon-based laser. In the core-shell nanowire laser design, the crystal phase control of wurtzite gallium arsenide (GaAs) nanowires enables the epitaxial growth of hex-SiGe shells.

Photoluminescence results indicate direct bandgap emissio [1], carrier confinement via quantum wells [2], and even amplified stimulated emission [3]. However, the realization of a coherent lasing signal remains elusive. Meanwhile, discrepancies between experiment and theory regarding carrier lifetime and recombination strength pose intriguing questions for further investigation of this novel material [4]. True understanding of Si and Ge in the hexagonal phase is hindered by insufficient material quality. Particularly, the interplay between I3 defect formation and growth rate leads to a snowball effect, increasing defect density with shell diameter [5].

We address this issue by improving our understanding of the growth dynamics near the GaAs-SiGe interface. By investigating shell growth in the 5-50 nm range, and analyzing the composition and growth temperature dependency, we identify adatom diffusion as the most critical parameter for suppressing defect formation. Using this knowledge, we achieve a significant reduction in I3 defect density, which is extended to more realistic shell diameters for nanowire laser geometries. The resulting material quality paves the way for further experimental exploration in the potential of hex-SiGe core-shell nanowires as silicon based laser, minimizing the impact of defects on their optical and electronic performance.

[1] E.M.T. Fadaly et al., *Nature* **580**, 205 (2020)
[2] W.H.J. Peeters et al*., Nat. Commun.* **15**, 5252 (2024)
[3] M.A.J. Van Tilburg et al., *Commun. Phys.* **7**, 328 (2024)
[4] C. Rödl et al., *Phys. Rev. Mater.* **3**, 034602 (2019)
[5] W.H.J. Peeters et al., *Phys. Rev. B* **111**, L241302 (2025)

Growing SiGe nanowires with the hexagonal phase

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Hexagonal phases of Ge and SiGe exhibit a direct bandgap and excellent light-emitting properties, with a tunable mid-infrared emission wavelength ranging from 1.8 to 4.2 µm for Si concentrations between 0 and 40% [1].

In previous work [2], we demonstrated that Au-catalyzed Ge nanobranches with a 2H crystal structure can grow epitaxially on the {1-100} sidewalls of GaAs wurtzite trunk nanowires, adopting the specific <1-100> growth direction (Figure 1.a) [1]. These Ge nanobranches maintain the 2H crystal structure under the Au catalyst. Depending on the growth conditions, an additional lateral layer of cubic Ge (3C) may also form on the (0001) facets, as illustrated in Figure 1.a.

Based on these findings, our objective is to grow hexagonal GeSi nanowires by ultra-high vacuum physical vapor epitaxy (UHV-PVE) on wurtzite bulk substrates with m-plane (1-100) surfaces. Since bulk wurtzite GaAs does not exist, we explored alternative substrates by first growing a GaAs buffer layer on hexagonal m-plane substrates with lattice constants compatible with Si and Ge, such as CdS-2H, ZnS-2H, and ZnS-4H (Figure1.b). This GaAs buffer layer then serves as a template for nanowire growth. We investigated the dewetting behavior of the Au catalyst and optimized the parameters for the growth of vertical hexagonal Ge and Ge/ $Si_{(1-x)}Ge_x$ nanowires with a composition of about x=0.55 (figure 1.c).

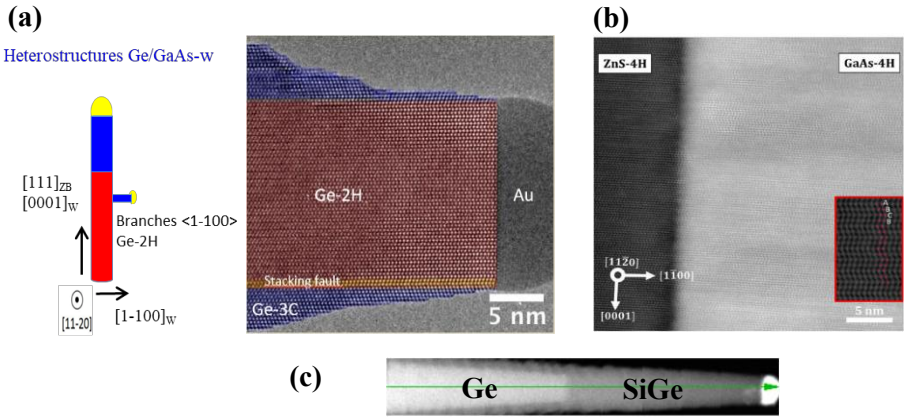

Fig. 1. (a) Representative schematic of the growth of a Ge-2H branch on a wurtzite GaAs nanowire trunk. The HR-TEM image shows the hexagonal 2H crystalline structure of the branch under the Au droplet and the presence of a cubic shell formed by lateral growth on the (0001) sidewalls. (b) STEM image along [11$\bar{2}$0] zone axis of the cross-section of the GaAs layer grown on a ZnS-4H substrate.(c) STEM image of $Si_{(1-x)}Ge_x$ heterostructure with an EDX linear scan showing the distribution of chemical elements along the nanowire.

[1] E.M.T. Fadaly et al., *Nature* **580**, 205 (2020)
[2] A. Li et al., *Nanotechnology* **34,** 015601 (2022)

Posters

Structural Characterization of $Cd_{1-x}Zn_xS$ Thin Films Grown on GaAs and on a- and m-plane Wurtzite CdS substrates by Metalorganic Chemical Vapor Deposition for the Synthesis of Hexagonal Si_xGe_{1-x} Layers

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Silicon (Si) and Germanium (Ge), which typically crystallize in the cubic diamond structure (3C), have long been fundamental materials in electronics. In recent years, metastable crystal phase engineering has emerged as a powerful technique for tuning electronic band structures and conduction properties, enabling new functionalities while maintaining chemical compatibility. Notably, the Si_xGe_{1-x} alloy in its hexagonal structure (2H) exhibits a direct bandgap (contrary to indirect cubic Si_xGe_{1-x}) and exceptional 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%. Despite recent progress, the synthesis of high-quality Ge-2H layers remains challenging. Until now, Ge-2H has been limited to nanostructures, core/shell nanowires [1], and nanobranches [2], restricting active volumes and hindering the scalability of device fabrication. To overcome this limitation, we propose the use of wurtzite (WZ) $Cd_{1-x}Zn_xS$ planar layers grown on WZ-CdS substrates as templates, as illustrated in the Figure 1. This could enhance the epitaxial growth of WZ-SiGe layers and enable the integration of this material into advanced optoelectronic devices. In this study, $Cd_{1-x}Zn_xS$ thin films were grown on GaAs (111) substrates and commercially available single-crystal CdS substrates with a-plane {1-100} and m-plane {11-20} orientations by

Metalorganic Chemical Vapor Deposition (MOCVD). This method offers advantages such as low growth temperature, high purity, and suitability for large-area deposition. However, one of the primary challenges lies in the surface preparation of CdS, which tends to oxidize and form stable surface oxides that are difficult to remove, thereby impeding epitaxy. The influence of both chemical and thermal pretreatments on the substrate surface was explored to improve interface quality. It was found that isopropanol effectively removes stains and most small particles by dissolving residues, facilitating their detachment. Efficient cleaning occurs at 500°C during annealing, while surface degradation begins at 550°C.The structural and morphological properties of the $Cd_{1-x}Zn_xS$ epitaxial layers were analyzed using X-Ray Diffraction (XRD) and Scanning Electron Microscopy (SEM).

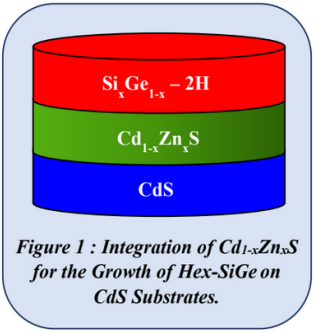

Figure 1 : Integration of $Cd_{1-x}Zn_xS$ for the Growth of Hex-SiGe on CdS Substrates.

[1] L. Vincent et al., *Adv. Mat. Inter.* **9-16**, 2102340 (2022)
[2] A. Li et al., *Nanotechnology* **34,** 015601 (2022)

Silicon germanium interdiffusion in hexagonal SiGe heterostructures

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The development of a silicon-based laser marks a key step toward realizing commercially viable photonic circuits. Among the most promising approaches are novel heterostructures composed of hexagonal silicon-germanium (hex-SiGe) grown on wurtzite gallium arsenide (GaAs) nanowires, which have demonstrated efficient direct band gap emission [1,2]. The band gap energy of SiGe can be tuned within the range of 0.35 to 0.65 eV through precise manipulation of the composition and quantum well (QW) thickness. However, a major challenge in realizing high-quality hex-/ QW systems lies in controlling Si-Ge interdiffusion, which can significantly alter the structural and electronic properties of heterostructures [3,4].

In this work, we investigate the impact of the thermal budget on SiGe/Ge QW systems. Therefore, we grow and anneal multiple QW structures around GaAs NWs and compare interdiffusion behavior in hexagonal (2H) and cubic (3C) crystal phases as a function of annealing time. Our results provide valuable insights toward optimizing multi-QW designs by balancing growth temperature and time to achieve high structural quality and compositional control.

We would like to especially thank funding from Europe's Horizon program OptoSilicon (964191), the Dutch foundation for Scientific Research (NWO), and the Bosch foundation.

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[4] W. Peeters, *Applied Physics and Science Education*, Eindhoven (2025).

Chemical Vapor Deposition Growth of Ge/Si-based Nanowire Heterostructures as Hole Spin Qubit Device Platforms

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Germanium (Ge)/Silicon (Si) nanowire (NW) heterostructures have been theoretically demonstrated to be some of the most promising candidates as device platforms for hole spin qubits in universal quantum computing applications [1,2]. This is due to their intrinsic high hole mobility, strong spin-orbit interaction, and low sensitivity to the noise caused by hyperfine interactions enabling ultrafast, all-electric, and high-fidelity read-out and control [1-3]. Various NW configurations have been proposed taking advantage of the carrier confinement and strain effects – Ge/Si core-shell NWs (CSNWs) [1,3], Si/Ge/Si curved quantum wells [2], and Ge/Si CSNWs with axial Si barriers [4]. For all of these heterostructures, strain is the key feature that strongly influences the hole spin behavior confined in quantum dots. In this work, we present the chemical vapor deposition growth and strain characterization of the three different NW heterostructure platforms in order to physically realize hole spin qubits. From our previous systematic work on the growth dynamics of Ge and Si Nws [5], the recipes and the corresponding parameters have been established in order to grow highly crystalline NWs with atomically sharp interfaces. Morphological and compositional characterization reveal highly crystalline growth of both the core and shell with sharp compositional interface indicating suppressed Si-Ge inter-diffusion. Moreover, strain effects have been qualitatively and quantitatively analyzed via geometric phase analysis and Raman spectroscopy, respectively. Lattice mismatch and strain analysis show that the growth of thicker shell exhibits more strain relaxation with respect to the core, while the core experiences increased strain with thicker shell. The established growth methods and the understanding of the corresponding strain paves the way for fabrication of Ge/Si NWs for the development of high performing hole spin qubits.

[1] C. Kloeffel, M. Trif, and D. Loss, *Phys. Rev. B* **84**, 1–8 (2011)
[2] S. Bosco and D. Loss, *Phys. Rev. Appl.* **18**, 1 (2022)
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[4] C. Y. Wen, M. C. Reuter, D. Su, E. A. Stach, and F. M. Ross, *Nano Lett.* **15**, 1654–1659 (2015)
[5] N. Forrer, A. Nigro, G. Gadea. and I. Zardo, *Nanomaterials* **13**, 1–13 (2023)

Empirical tight-binding Hamiltonian for cubic and hexagonal Ge: parametrisation from first-principles calculations

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The group-IV semiconductor germanium (Ge) possesses an indirect band gap in its conventional diamond (cubic, 3C) crystal phase but, when grown in the metastable lonsdaleite (hexagonal, 2H) phase, Ge possesses a direct band gap. However, the predicted radiative recombination rate of 2H-Ge is low [1], motivating exploration of strain and heterostructuring to enhance optical emission.

The predicted presence of type-I band offsets between 2H-Ge and 3C-Ge presents the possibility to realise direct-gap 2H/3C-Ge polytype heterostructures (PHs) [2]. PHs are monomaterial quantum wells – 2H-Ge "wells" surrounded by 3C-Ge "barriers" – realised by alternating the crystal phase along the [111]/[0001] axis. The development of Ge PHs containing both 3C-Ge and 2H-Ge has the potential to engineer the electronic band structure for applications spanning classical and quantum photonic and electronic devices [3]. The length scales relevant to device applications can push PH simulations beyond the reach of first-principles density functional theory (DFT) calculations. This mandates development of "transferable" empirical atomistic models that can accurately describe the electronic structure of a given material in its distinct (meta)stable phases. The empirical tight-binding (ETB) method is computationally inexpensive, but transferable ETB models have been challenging to realise in practice [4].

We develop an ETB Hamiltonian that prioritises transferability between the 3C and 2H phases, which both possess fourfold (tetrahedral) coordination. We begin with a $sp^3d^5s^*$ ETB Hamiltonian for 3C-Ge, and seek transferability by modifying the Hamiltonian to account for local changes in crystal structure between the 2H and 3C phases. The ETB Hamiltonian is parametrised via hybrid functional DFT electronic structure calculations for 3C-Ge and 2H-Ge using a fitting procedure that, in addition to considering the band dispersion, also explicitly accounts for the orbital character of the wave functions. The results of DFT and ETB electronic structure calculations for exemplar 2H/3C-Ge PHs are compared to assess the quality of the ETB Hamiltonian. The establishment of an accurate transferable ETB model for Ge provides a basis for inexpensive predictive calculations of technologically-relevant properties in heterostructured Ge nanowires, paving the way for in silico design of novel device structures.

[1] C.A. Broderick, X. Zhang, M. E. Turiansky, and C.G. Van de Walle, arXiv:2412.08865 (2024)
[2] T. Kaewmaraya, L. Vincent, and M. Amato, *J. Phys. Chem. C* **121**, 5820 (2017)
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[4] C A. Broderick, E.P. O'Reilly and S. Schulz, *J. Appl. Phys.* **135**, 100902 (2024)

Pressure-dependent kinetics of phase transitions in Si and Ge using machine learning interatomic potentials

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Silicon (Si) and Germanium (Ge) exhibit several metastable phases promising for the integration of optoelectronics into Si-based devices. In particular, the hexagonal diamond (*hd*) phase of Ge has been shown to exhibit a direct band gap [1]. These metastable phases can be synthesised starting from the most stable diamond cubic (*dc*) phase by a series of pressure-induced phase transitions via nanoindentation.

Here we show how we explored pressure-induced phase transitions in silicon by advanced modeling techniques based on established ML potentials. We performed large-scale Molecular Dynamics (MD) simulations [2], coaudivated by a Neural Network-based tool for the on-the-fly phase identification (as shown in Fig. 1). We also studied the kinetics of the atomistic mechanisms underlying phase transitions by Potential Energy Surface exploration methods like the Nudged Elastic Band (NEB) and the Dimer method [3]. We reveal the competition between local nucleation events and full-cell transitions by a synergic exploitation of pressure-controlled MD simulations and the study of kinetics of phase transitions by NEB [4].

Furthermore, we also developed a ML interatomic potential specifically tailored for the study of kinetics of pressure-induced phase transitions in Ge [2]. We demonstrate how this potential enables detailed exploration of the kinetics of phase transitions, and we tested its performance on dynamical properties like phonon spectra and frequency prefactor calculations.

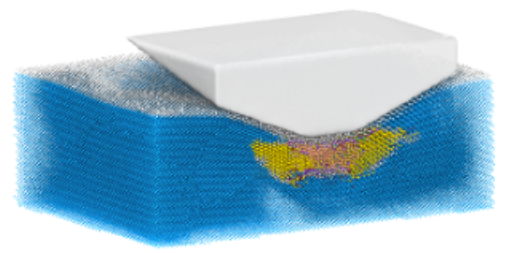

Fig. 1. Large-scale MD simulation of the nanoindentation process. Several pressure-induced phase transitions starting from the dc substrate (in blue in the figure) can be observed during the simulation and are highlighted in the figure by different colors.

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TEM analysis of Textured Silicon Polymorph Crystals obtained via Nanoindentation and Annealing

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Silicon polymorphs exhibit unique properties, such as the combination of low thermal conductivity with high thermoelectric efficiency, or high carrier mobility with superconductivity. Some polymorphs are also predicted to possess a direct bandgap. Among these, hexagonal (hd) silicon is particularly attractive due to its potential use as a template for the epitaxial growth of hexagonal SiGe alloys. These alloys can maintain a tunable direct bandgap across a broad compositional range, offering significant flexibility for optoelectronic applications.

In our recent work [1], we demonstrated the formation of micrometer-sized, textured hexagonal silicon crystals through nanoindentation followed by rapid post-indentation annealing. This approach offers a simpler alternative to more complex synthesis methods, such as those involving nanowires or sophisticated deposition systems. Under mechanical pressure, diamond cubic silicon (dc-Si) transforms into a metallic β-Sn phase (Si-II) at high pressures. Upon pressure release, and by optimizing the nanoindentation unloading process, we observed—via Raman spectroscopy—the formation of a mixed body-centered cubic (bc8, Si-III) and rhombohedral (r8, Si-XII) phase.

In this study, we investigate nanoindented diamond cubic silicon (100) pits prior to annealing to gain deeper crystallographic insight into the intermediate metastable Si phases. The system was analyzed using advanced characterization techniques, including polarized Raman spectroscopy and transmission electron microscopy (TEM). TEM micrographs revealed extensive regions of r8/bc8 phases well-aligned with the Si (001) substrate. As an alternative to rapid annealing for producing hexagonal silicon, we also explored the effects of slow annealing. This process led to the formation of other polymorphs, potentially attributable to Si-XIII, a phase with an as-yet unidentified crystal structure.

The authors acknowledge financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 104 published on 2.2.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union – NextGenerationEU– Project Title ”SiGe Hexagonal Diamond Phase by nanoIndenTation (HD-PIT)” – Prot. 2022EYXJ5X – CUP B53D23004120006 (CUP Master H53D23000780001) – Grant Assignment Decree No. 957 adopted on 30.06.2023 by the Italian Ministry of Ministry of University and Research (MUR).

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Pseudo-substrates, based on m-plane ZnS, for hexagonal SiGe growth

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One difficulty in growing hexagonal Ge or SiGe is the lack of well adapted substrates. ZnSe and GaAs would be the best candidates, with a limited lattice mismatch, typically 1 to 2%, along the **a** as well as the **c** axis. Unfortunately, excepted in some nanostructures, ZnSe and GaAs are available only in their cubic form. The rare commercially available hexagonal substrates, CdSe or CdS exhibit a larger mismatch, up to 7%. Although ZnS does exist in the wurzite phase, it is not commercially available in the form of the required m-plane substrates.

This work aims to develop pseudo-substrates of m-plane GaAs or ZnSe, by growing relaxed layers of these compounds, by molecular beam epitaxy (MBE), on m-plane ZnS substrates. As noted above, such substrates are not yet commercially available. The first step in this process was then to extract, from a bulk crystal, thin slabs of ZnS accurately oriented along the required m-plane, and carefully polished mechanically to achieve a fine roughness of 2 nm RMS. After cleaning, the last step consisted in a chemical attack using diluted Br-methanol to remove the thin surface layer damaged by polishing and to complete the surface smoothing.

Various growth approaches were considered, including MBE versus MEE (Migration Enhanced Epitaxy). MEE consists in providing Se (resp. As) continuously while Zn (resp. Ga) is supplied by periodic pulses. Regarding ZnSe grown on ZnS, our best results (fig. 1) were obtained by MEE at 400°C. In the case of MBE growth, the results under Se excess are clearly better than under Zn excess. Regarding GaAs on ZnS, our best results (fig. 2) were obtained by MBE, at 500°C, under high arsenic excess: the arsenic beam equivalent pressure is set 20 times higher than the gallium one. Our growth conditions for GaAs still need improvement compared to those of ZnSe.

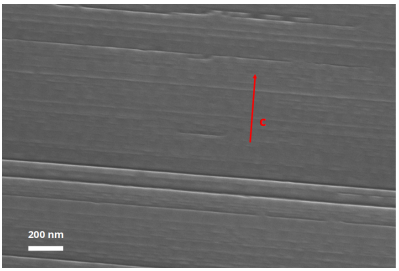

Fig. 1. SEM of ZnSe, on m-plane ZnS, grown by MEE

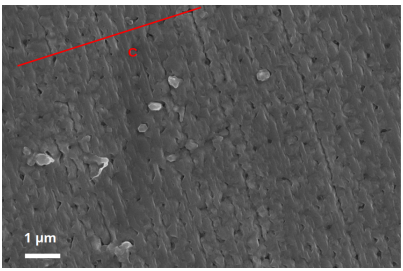

Fig. 2. SEM of GaAs, on m-plane ZnS, grown by MBE.

In our best ZnSe layers, the SEM images suggest a strongly anisotropic structural quality of the epitaxial layer. This is confirmed by the X-ray diffraction study (not shown here) which furthermore indicates that the structural quality of our initial ZnS bulk crystal is also weak and anisotropic. New substrates are currently being prepared from different ingots to distinguish between defects inherited from the substrate and any lack of optimisation in the growth conditions.

Preliminary trials of pseudo-substrates grown by MEE on commercial CdS and CdSe m-plane substrates will also be presented.

Electronic and Optical Properties of Hexagonal SiGe and GeSn Alloys: A Combined First-Principles and k·p Investigation

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We present ab initio calculations for bulk hexagonal $Ge_{1-x}Sn_x$ alloys. Our findings confirm that hexagonal GeSn is a direct-bandgap semiconductor over a wide composition range, making it an interesting material for optoelectronic applications in the infrared region. We systematically investigate the dependence of the fundamental band gap, effective masses, and optical transition on Sn content.

Building on these first-principles results, we expand our previously developed k·p theory for pure hexagonal Ge[1]. The ab initio calculations provide the robust parameterization needed to reliably extend this powerful semi-empirical model to group-IV alloys. We apply this extended methodology to hexagonal $Si_{0.25}Ge_{0.75}$, a system of significant current interest. Our analysis reveals a massive enhancement in the optical transition strength at the fundamental direct gap. This key finding, first shown via our direct Density Functional Theory (DFT) calculations, is also successfully reproduced by our extended k·p model. This points to significantly increased light absorption and emission efficiency, highlighting the exceptional potential of hexagonal SiGe alloys for high-performance photonic devices.

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Integration of Hex-SiGe into a NW-induced Photonic Crystal Cavity

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Cubic silicon (Si) is an indirect bandgap semiconductor and is therefore known for being an inefficient light emitter. In contrast, hexagonal SiGe (Hex-SiGe) has been shown to exhibit a direct bandgap for a Ge content exceeding 67%. Since Si and Ge naturally crystallize in the cubic phase, Hex-SiGe is synthesized as a shell around a wurtzite (WZ) GaAs NW core using the crystal transfer method. By varying the Ge content, the emission wavelength can be tuned across a broad spectral range from 1.8 to 3.4 µm [1]. As a step towards realizing a Hex-SiGe laser, individual NWs lying on an AlN substrate have been investigated and were shown to exhibit amplified spontaneous emission. Hakki-Paoli analysis indicates that reflection losses of the Fabry-Perot resonator significantly contribute to overall cavity losses with geometrical Q-factors around 60. This suggest that conventional mirror-based feedback is insufficient for effective confinement [2]. To address this, we aim at enhancing optical feedback by embedding the NW within a silicon photonic crystal slot waveguide cavity [3].

We demonstrate a fabrication technique to manipulate individual Hex-SiGe NW into the slot waveguide (fig. 1a) using a PDMS/PC transfer printing approach as well as a systematic investigation of the self-localized resonant modes emerging from a comparable dielectrically loaded slot waveguide cavity through introducing a Si segment in top-down fabrication (fig. 1b). Cross-polarized reflectance spectroscopy has provided valuable insights into optimizing photonic crystal cavities for mid-infrared wavelengths. For our application, the resonance energy can be tuned within the range of 0.465 eV to 0.61 eV by adjusting lattice constant and hole radius to cover the full emission range of Hex-Si0.2Ge0.8. Our findings indicate that the optical modes are predominantly determined by the photonic crystal geometry rather than the segment geometry, as evidenced by the limited sensitivity to changes in segment length and position (fig. 1c). For longer segments, we observed higher order PhC cavity modes and studied their spatial overlap with the segment (fig. 1d).

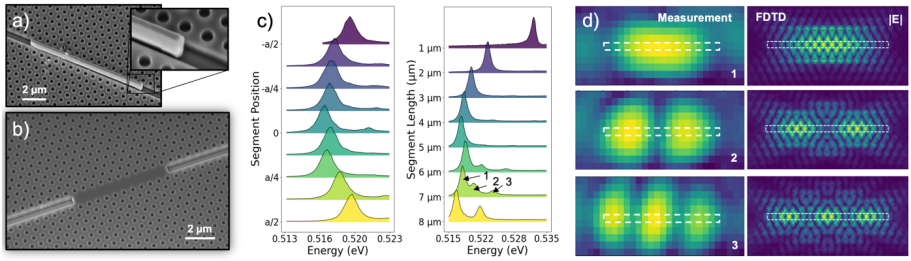

Fig. 1. a) SEM image of a Hex-SiGe NW transferred into the slot waveguide cavity. b) Top-down etched Si segment allowing systematic studies of resonant modes. c) spectra from cross-polarized reflectance spectroscopy indicate low susceptibility of cavity modes to segment position and segment length. d) Measurements of spatially resolved mode profiles of a 7 µm long segment (as indicated in fig. 1c) compared to FDTD simulations.

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Exploring Spin Dynamic Properties of Direct-Bandgap Hex-SiGe for On-Chip Silicon Photonics Applications

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In the quest for advancing quantum technologies, silicon quantum dots have long been recognized as a favorable host for spin qubits due to their stability, availability of nuclear spin-free isotopes, and compatibility with modern semiconductor technology. The indirect bandgap of cubic silicon, however, suppresses efficient optical interactions and hinders the realization of a spin–photon interface [1]. In contrast, hexagonal SiGe (Hex-SiGe) has been recently demonstrated to exhibit a direct bandgap when the Ge content exceeds 67%, enabling efficient and tunable light emission in the 1.8–3.4 µm range [2]. Such combination of spin coherence in the silicon platform and optical accessibility in Hex-SiGe highlights its potential for bridging electronic spins and photons [3]. Nevertheless, as a relatively new material system, critical questions remain regarding its ability to confine electron spins and enable their optical control, making a thorough understanding of its spin dynamics essential.

In our research, we aim to characterize the spin dynamics in hex-SiGe nanowires by combining time resolved and Hanle effect measurements [4]. Hereby, we will apply near-resonant excitation with tunable continuous wave (CW) laser and probe the magnetic field dependent degree of polarization of emitted light induced by optical orientation. Together with time-resolved photoluminescence measurements to determine the radiative lifetime, this approach allows extraction of the g-factor and spin relaxation in Hex-SiGe. We anticipate that measurements as a function of lattice temperature, carrier and impurity density will elucidate the mechanisms responsible for spin relaxation. To this end, we have constructed a MIR micro-PL setup allowing the measurement of Hanle curves for Hex-SiGe nanowires emitting close to 2.3 µm (fig 1a) and typical polarization resolved data recorded from InAs NWs is presented in (fig 1b).

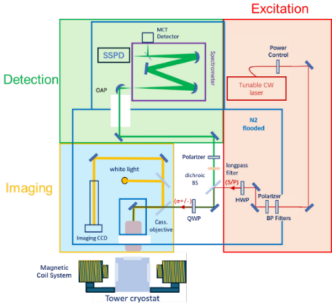

Fig. 1a. Optical setup for Hanle effect measurement. The sample is placed in a He-free cryostat and accessed via imaging system. A tunable CW laser excites the sample, while the PL signal is detected by the SSPD. A transverse magnetic field depolarizes the optically induced spin population.

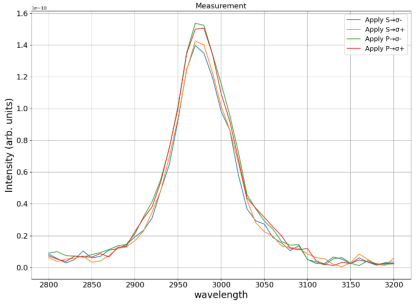

Fig. 1b. Typical PL emission from bulk InAs sample excited by 4 different polarization configurations. With non-resonant excitation, no optical orientation is observed and all configurations give similar response.

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Hexagonal Germanium Nanowires as a Spin Qubit Platform

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Hexagonal germanium (2H-Ge) has recently emerged as a promising candidate for spin qubit applications, offering a unique combination of strong spin–orbit interaction and optical activity [1]. Recent advances in growing hexagonal Si_xGe_{1-x} nanowires with controlled dimensions and tunable compositions provide experimental pathways to realize such quantum structures [2]. Unlike conventional spin qubit host materials such as GaAs, cubic Si, and cubic Ge, hexagonal Ge is expected to enable direct bandgap transitions and enhanced qubit control via optical coupling, making it a compelling platform for scalable quantum technologies. In this work, we investigate the electronic and spin properties of 2H-Ge nanowires using a multiband **k·p** Hamiltonian proposed by Pulcu et al. [3], which effectively captures the low-energy band structure near the point. By discretizing this Hamiltonian and implementing open boundary conditions in the transverse directions, we construct a nanowire model oriented perpendicular to the c axis. We analyze the resulting band structure and confinement-induced gap variations as a function of nanowire cross-sectional size and transverse electric field. Furthermore, we incorporate magnetic field effects via Peierls substitution to study the anisotropic response of the nanowire under longitudinal and transverse magnetic fields. This allows us to calculate and examine the modulation of the effective g-tensor across different field orientations. Our results reveal direction-dependent shifts in spin splitting and effective g-factors, offering insights into optimal qubit operation regimes in hexagonal Ge-based systems. These findings may guide device fabrication using existing hexagonal SiGe nanowire growth techniques [4].

This research is supported by the European Union within the Horizon Europe research and innovation programme via the ONCHIPS project under grant agreement No 101080022, and by the HUN-REN Hungarian Research Network through the Supported Research Groups Programme, HUN-REN-BME-BCE Quantum Technology Research Group (TKCS-2024/34). We also acknowledge funding from the National Research, Development and Innovation Office of Hungary under OTKA grant no. FK 146499.

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[2] D. Lamon et al., *Nano Lett.* **25**, 14, 5741–5746 (2025)
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[4] A. Li et al., *Nanotechnology* **34**, 015601 (2022)

Realization of Ohmic Contacts on hexagonal SiGe Nanowires

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In recent years, extensive research has been done on semiconducting materials in order to bridge the gap between photonic and conventional electronic semiconductor devices. Combining both worlds in the same material system would result in novel spin-photon interfaces and open up exciting new possibilities for quantum computing. Due to silicon (Si) and germanium (Ge) being the industry standard regarding electronic semiconducting devices - but unfortunately in their cubic (3C) phase with an indirect band gap - a lot of effort has been put into investigating whether a direct band gap in these two main material systems could be realized. With successful growth of hexagonal (2H) Si/Ge nanowires (NWs) the first steps towards direct band gap Group IV semiconducting devices has been achieved [1-5].

Here, we report on the electronic characterization of 2H-SiGe NW field effect transistors (FETs). In particular, we investigate for different SiGe-alloy compositions which metal is best suited as electrode material in order to achieve Ohmic contacts, as this paves the way to build more complex devices, such as double quantum dots, and investigate spin qubit physics in this novel direct band gap semiconducting material [6-8].

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[8] M. Brauns, et al., *Appl. Phys. Lett.* **109**, 143113 (2016)

Crystallography of silicon element: stable and metastable crystalline forms

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HP research on Si started more than 50 years ago and since then several allotropes, displaying a wide variety of physical properties, have been reported. The narrow-bandgap semiconductor Si-III with BC8 structure (originally believed to be semimetal) can be obtained from the high-pressure tetragonal metallic phase, Si-II, formed during compression of common silicon according to Si-I→Si-II. Such a transformation during decompression can be either direct, Si-II→Si-III, or with an intermediate step Si-II→Si-XII→Si-III. Our in situ studies of pure Si in oxygen-free environment indicated that in the absence of pressure medium, Si-I remains metastable at least up to ~14 GPa, while the pressure medium allows reducing the onset pressure of transformation to ~10 GPa. Upon heating Si-III at ambient pressure a hexagonal structure, named Si-IV, was observed. This allotrope was believed to be a structural analogue of the hexagonal diamond found in meteorites (called also lonsdaleite) with the 2H polytypestructure. Calculations have predicted several hexagonal polytypes of Si and of other Group-IV elements to be metastable, such as 2H (AB), 4H (ABCB) and 6H (ABCACB). Exhaustive structural analysis, combining fine-powder X-ray and electron diffraction, afforded resolution of the crystal structure. We demonstrate that hexagonal Si obtained by high-pressure synthesis correspond to Si-4H polytype (ABCB stacking), in contrast with Si-2H (AB stacking) proposed previously. The sequence of transformations Si-III→Si-IV(4H)→Si-IV(6H) has been observed in situ by powder X-ray diffraction. This result agrees with prior calculations that predicted a higher stability of the 4H form over 2H form. Further physical characterization, combining experimental data and ab-initio calculations, have shown a good agreement with the established structure. Strong photoluminescence emission was observed in the visible region, for which we foresee optimistic perspectives for the use of this material in Si-based photovoltaics. The study of silicon allotropic transformation in Na-Si and K-Si systems at high pressure, high temperature conditions indicated new interesting results on the second-order character of Si-II→Si-XI transformation and will be discussed in the presentation. The impact of the second order character on the topology of the pressure-temperature phase diagram of silicon will be analyzed.

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