

4TH INTERNATIONAL WORKSHOP

Hexagonal SiGe and Related Materials

14–15 September 2026

Amphitheatre, Vrijhof
University of Twente, Enschede
The Netherlands



Organised by the European project
ONCHIPS

THE WORKSHOP AT A GLANCE

Dates	Monday 14 – Tuesday 15 September 2026
Venue	Amphitheatre, Vrijhof (building 47) University of Twente, Enschede
Dinner	Monday 18:15, Het Paradijs, Enschede Bus leaves the U Parkhotel car park at 17:50
Posters	Monday 12:15–14:00, with lunch
Contact	hexsige@utwente.nl
Website	www.hexsige26.eu

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Practical information

The essentials for both days.

REGISTRATION

Registration opens at 08:30 on Monday in the Vrijhof, with coffee and tea. On Tuesday the walk-in, again with coffee and tea, also starts at 08:30. The staff at the Vrijhof service desk will point you to the Amphitheatre.

LECTURE HALL

All sessions take place in the Amphitheatre of the Vrijhof, building 47 on the campus map.

TALKS

Invited lectures have 40-minute slots and contributed talks 20-minute slots.

POSTERS

The poster session is on Monday from 12:15 to 14:00, together with lunch and the group photograph. Posters can go up during the Monday morning coffee break and are taken down in the Tuesday morning break. The abstracts in this booklet carry the numbers P1 to P16, in the order of the poster section.

MEALS

The registration fee includes the workshop itself, the lunches, refreshments during the coffee breaks, and the workshop dinner. Lunch is served on Monday from 12:15 to 14:00, alongside the posters, and on Tuesday from 12:45 to 14:00 after the closing.

WORKSHOP DINNER

The dinner is on Monday evening at Het Paradijs in Enschede. A bus leaves the U Parkhotel car park at 17:50 and returns to the campus after dinner, which runs from 18:15 to 21:00. The address and what to do if you miss the bus are on page 17.

WI-FI

eduroam is available on the campus.

FINDING YOUR WAY

Travel directions start on page 11, the campus map is on page 13, and the venue, the hotels and the dinner restaurant, with their addresses, are on page 15.

Buses	9292.nl
Trains	ns.nl/en/journeyplanner
Campus map	utwente.nl/campusmap

IN AN EMERGENCY

For an emergency on campus, call University Security on **+31 53 489 2222**; for the national emergency services, call **112**. Security and the Infocentre are in the Spiegel, building 2. The Medical Centre, building 58, has a doctor and a dentist.

CONTACT

Email	hexsige@utwente.nl
Website	www.hexsige26.eu
U Parkhotel	+31 53 433 13 66
Intercity Hotel	+31 53 207 0000

The programme in this booklet is the definitive version of 1 September 2026. The programme is also published on www.hexsige26.eu.

Programme

All sessions take place in the Amphitheatre of the Vrijhof (building 47). The page number beside a talk points to its abstract.

DAY ONE

Monday 14 September

Amphitheatre, Vrijhof

08:30 – 09:00 Registration, coffee and tea

09:00 – 09:10 **Welcome and opening**
Floris Zwanenburg, University of Twente

09:10 – 10:40 MATERIALS AND DEVICES I

Chair: Jonathan Finley, TU Munich

09:10 **Caspar van der Wal**
INVITED University of Groningen
Spin-active colour centres: the case of transition-metal impurities in 4H-SiC

09:55 **Anirban Das**
Budapest University of Technology and Economics
Spin-orbit interaction and g-tensor anisotropy of holes in nanowires of hexagonal germanium [p. 28](#)

10:20 **Guido Wiersma**
University of Twente
Electronic characterisation of hex-SiGe/Si core/shell nanowires [p. 30](#)

10:40 – 11:10 Coffee break, put up posters

11:10 – 12:15 MATERIALS AND DEVICES II

Chair: Jonathan Finley, TU Munich

11:10 **Stefano Bosco**
INVITED TU Delft
Spin-orbit engineering in Ge for quantum computing

11:55 **Enrico Degan**
Walter Schottky Institute, TU Munich
Non-linear optical spectroscopy of hexagonal SiGe alloys [p. 31](#)

12:15 – 14:00 Group photograph, lunch and poster session

14:00 – 15:30 THEORY AND QUANTUM PROPERTIES I

Chair: Jos Haverkort, TU Eindhoven

14:00

Christopher Broderick

University College Cork

INVITED*Theory of optical gain and alloying in hexagonal-Ge-based semiconductors*

14:45

Perpetua Muchiri

Université Paris-Saclay, CNRS, Orsay

DFT-1/2 study of the effects of intrinsic defects on the electronic structure of silicon polytypes p. 33

15:10

Veronica Regazzoni

University of Milano-Bicocca

Structural defects in planar hexagonal Ge: from HR-TEM observations to atomistic simulations p. 34

15:30 – 16:00

Coffee break and posters

16:00 – 17:30 GROWTH, SYNTHESIS AND EPITAXY I

Chair: Erik Bakkers, TU Eindhoven

16:00

Giovanni Isella

Politecnico di Milano

INVITED*Deposition of planar 2H-Ge on CdS by low-energy plasma-enhanced CVD*
p. 36

16:45

Alexandre Courac

IMPMC, Sorbonne Université

Hexagonal Si polytype 6H by in situ synthesis p. 38

17:10

Denny Lamon

TU Eindhoven

Branched nanowires for quantum dots and core-shell structures p. 39

17:50

Bus leaves from the U Parkhotel car park for Enschede city centre

18:15

Workshop dinner at Het Paradijs (see p. 17)

21:00

Bus returns to the campus

DAY TWO

Tuesday 15 September

Amphitheatre, Vrijhof

08:30 – 09:00 Walk-in, coffee and tea

09:00 – 10:30 **SYNTHESIS AND EPITAXY II**

Chair: Giovanni Isella, Politecnico di Milano

09:00

Bernardette Kunert

INVITED

IMEC, Leuven

Challenges and opportunities in III–V device integration to silicon photonics

09:45

Santhanu Panikar Ramanandan

TU Eindhoven

Planar epitaxy of direct band gap hexagonal germanium layers p. 41

10:10

Fabrizio Rovaris

University of Milano-Bicocca

Role of the metastable Si-XIII structure in the diamond-to-hexagonal phase transition p. 42

10:30 – 11:00 Coffee break, take down posters

11:00 – 12:30 THEORY AND QUANTUM PROPERTIES IIChair: Jos Haverkort, TU Eindhoven

11:00

Michele Amato

CNRS, Université Paris-Saclay

INVITED*Defects, doping and phase engineering in hexagonal-diamond silicon*

11:45

Mette Schouten

TU Eindhoven

Growth kinetics of hex-SiGe on wz-GaAs core nanowires p. 44

12:10

Yetkin Pulcu

University of Konstanz

Structural, electronic and optical properties of hexagonal GeSn from density functional theory p. 45

12:35 – 12:45

Closing

Floris Zwanenburg, University of Twente

12:45 – 14:00

Lunch

Getting there

The campus lies between Enschede and Hengelo. Bus, train, car and plane, one route at a time.

The venue is the **Vrijhof**, building 47 on the University of Twente campus. The campus address for navigation is **De Veldmaat 5, 7522 NM Enschede**. Two bus stops serve the campus from the south side: *Enschede Kennispark/UT* and *Enschede Westerbegraafplaats/UT*.



By train

Enschede is the eastern terminus of the Dutch intercity network. Take a train to **Hengelo**, **Enschede** or **Enschede Kennispark**, then follow the bus directions below. Trains between Enschede and Enschede Kennispark run at least twice an hour. From Enschede Kennispark you can also walk onto the campus in 15 to 20 minutes, depending on where you need to be.

From Germany: Enschede has a German platform with services to Coesfeld, Münster and Dortmund. If you take the Berlin–Amsterdam intercity instead, get off at Hengelo.

Journey planner: ns.nl/en/journeyplanner



By bus

Both bus lines run frequently and stop on or beside the campus.

- **From Hengelo station:** bus **9** towards Enschede. Get off at Kennispark or Westerbegraafplaats/UT.
- **From Enschede station:** bus **1** towards Universiteit (stops on the campus itself), or bus **9** towards Hengelo, getting off at Kennispark or Westerbegraafplaats/UT.
- **From Enschede Kennispark station:** bus **1** towards Universiteit.

There are several stops on the campus; they are marked on the map overleaf. Extra services run during peak hours.

Journey planner: 9292.nl



By car

Enter **De Veldmaat 5, 7522 NM Enschede** into your navigation system, then follow the signs on campus to the Vrijhof. There is a car park at the U Parkhotel, building 45, close to the venue; it is labelled on the campus map on page 13. At the Vrijhof service desk the staff will point you to the Amphitheatre.



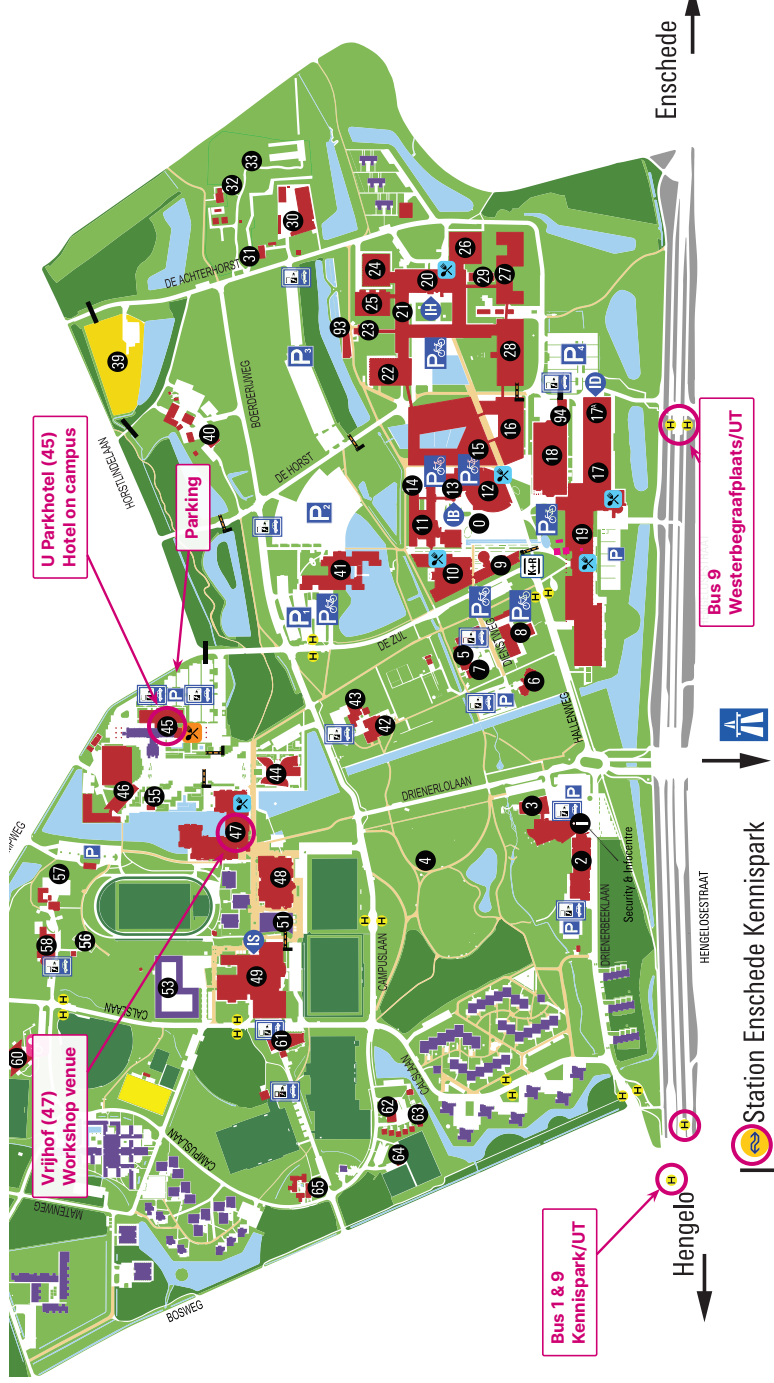
By plane

Fly into **Amsterdam Schiphol (AMS)**, the main Dutch airport. An intercity train runs from beneath the terminal via Amersfoort to Enschede, twice an hour, taking about two hours. Get off at Hengelo or Enschede and continue by bus as above.

Public transport in the Netherlands is contactless: tap in and tap out with a bank card or phone at the card readers on the bus and at the station gates. If you forget to tap out, you are charged a maximum fare.

University of Twente campus

Building numbers match the signs on campus.



47 Vrijhof

The venue. All sessions are in the Amphitheatre; the service desk will point you to it.

45 Hogekamp

U Parkhotel and its restaurant. The car park next to it is where the dinner bus leaves from.

Kennispark/UT

Bus 1 and 9 stop here. The train station is just south of the main road.

Westerbegraafplaats/UT

Bus 9 stops here, at the south-east edge of the campus.

The buildings

The venue, the hotels, and the dinner restaurant.



Vrijhof

VENUE • BUILDING 47

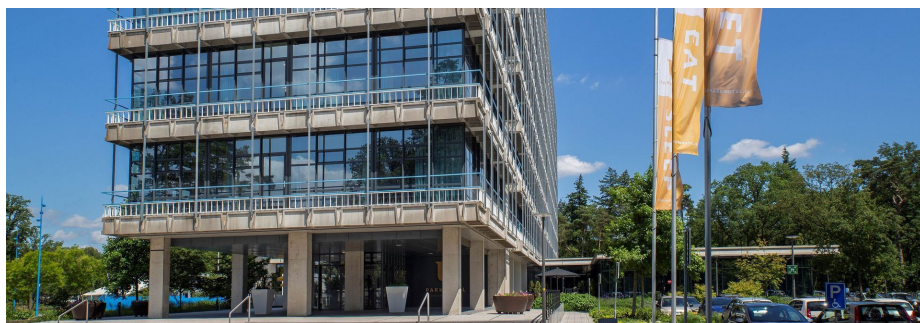
De Veldmaat 5
7522 NM Enschede

All sessions take place in the **Amphitheatre** of the Vrijhof. Go in through the main entrance; the staff at the service desk will point you the right way.

From Enschede Kennispark station you can walk to the campus in 15 to 20 minutes, depending on where you need to be.



The Amphitheatre, where all sessions take place.

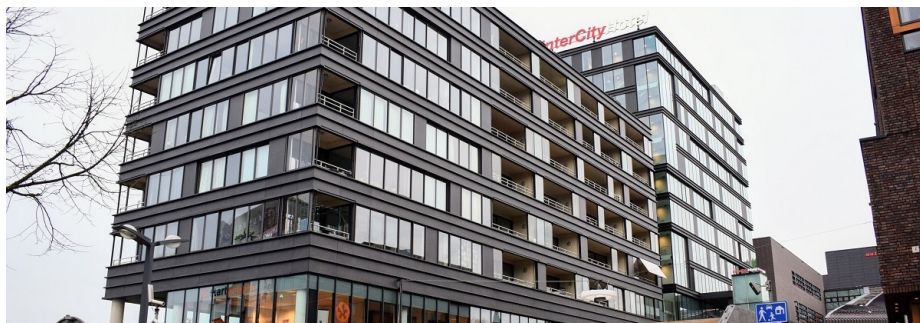


U Parkhotel

HOTEL • BUILDING 45, HOGEKAMP

De Veldmaat 8
7522 NM Enschede
+31 53 433 13 66

The hotel is on the campus itself, in the Hogekamp building, a short walk from the Vrijhof. The building also houses the U Parkhotel restaurant and Campus 053.



IntercityHotel Enschede

HOTEL • CITY CENTRE

Willem Wilminkplein 5
7511 PG Enschede
+31 53 207 0000

In the centre of Enschede, close to the main railway station. From Enschede station, take bus 1 towards Universiteit or bus 9 towards Hengelo to reach the campus; trains between Enschede and Enschede Kennispark run at least twice an hour.



Het Paradijs

WORKSHOP DINNER • MONDAY EVENING

Nicolaas Beetsstraat 48
7514 CW Enschede

Het Paradijs is a special and relaxing place: good food in a green, almost magical setting, a little outside the centre of Enschede.

A bus leaves the U Parkhotel car park at 17:50 and brings everyone straight there; dinner runs from 18:15 to 21:00, and the bus returns to the campus afterwards. If you miss it, take bus 9 to Enschede city centre; from there it is about a 15-minute walk.

Invited speakers

Six lectures over the two days, in the order they appear in the programme.

Caspar van der Wal

University of Groningen

Spin-active colour centres: the case of transition-metal impurities in 4H-SiC



Caspar van der Wal obtained his PhD in 2001 with Hans Mooij at Delft University of Technology, on the quantum coherent dynamics of superconducting circuits, and continued as a postdoc at Harvard University working on quantum optical memories in atomic vapours. He is now full professor in Physics of Quantum Devices at the Zernike Institute for Advanced Materials in Groningen, where his team explores spintronic and quantum-information functionalities with electron and nuclear spins in semiconductor devices, using both quantum optical and electron transport methods. Since 2009 he has served as education director or scientific director at the Zernike Institute.

Stefano Bosco

TU Delft

Spin-orbit engineering in Ge for quantum computing



Stefano Bosco leads a group working on the theory of semiconducting quantum computing, with an emphasis on spin qubits and quantum devices, combining microscopic modelling with hardware-oriented approaches in close collaboration with experimental teams. He studied nanoelectronics engineering at Politecnico di Milano and completed graduate studies at KU Leuven and Chalmers University of Technology, before earning his PhD with distinction at RWTH Aachen University and Forschungszentrum Jülich under David DiVincenzo. After postdoctoral and staff scientist positions at the University of Basel with Daniel Loss, he now develops next-generation quantum device architectures.

Christopher Broderick

University College Cork

Theory of optical gain and alloying in hexagonal-Ge-based semiconductors



Chris Broderick received his PhD in Physics from University College Cork, after which he held postdoctoral appointments at the University of Bristol and the Tyndall National Institute. From 2021 to 2023 he was a Marie Curie Global Fellow at the University of California, Santa Barbara, and in 2024 he was awarded a Royal Society University Research Fellowship. Since 2025 he has been Lecturer (Associate Professor) in Quantum & Photonics at the School of Physics at University College Cork.

Giovanni Isella

Politecnico di Milano

Deposition of planar 2H-Ge on CdS by low-energy plasma-enhanced CVD



Giovanni Isella is Full Professor of Semiconductor Physics at the Politecnico di Milano, where he leads the SiGe epitaxy team. Since 2001 he has exploited strain and band-gap engineering of SiGe heterostructures across a range of applications, including near- and mid-infrared integrated photonics (SiGe waveguides and multiple quantum well modulators), thermoelectric energy conversion in low-dimensional systems, spintronics in Ge heterostructures, and hole-based qubits.

Bernardette Kunert

IMEC, Leuven

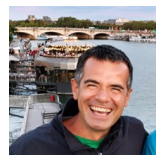
Challenges and opportunities in III–V device integration to silicon photonics

Bernardette Kunert received her Dr. rer. nat. in Physics from the University of Marburg in 2005. After working as a project manager in a start-up from 2006, she joined imec in Belgium as a Principal Scientist in 2013, and has been Scientific Director since 2023. She has a strong background in the epitaxial growth and characterisation of III–V heterostructures and related (opto)electronic devices, with a central theme of integrating III–V functionality onto large-diameter silicon or germanium substrates. In her current role she is jointly responsible for defining imec's III–V technology strategies.

Michele Amato

CNRS, Université Paris-Saclay

Defects, doping and phase engineering in hexagonal-diamond silicon



Michele Amato is Associate Professor at the Laboratoire de Physique des Solides, Université Paris-Saclay. He received his PhD in Physics from the Università di Modena e Reggio Emilia in 2011, and after research stays at the Institut de Ciència de Materials de Barcelona and at the LPS in Orsay was awarded a Marie Curie Fellowship at the École Polytechnique in Paris. From 2013 to 2019 he was Assistant Professor at Université Paris-Sud. His research focuses on first-principles simulations of semiconductors and nanostructures, particularly defects, doping and optical properties in group-IV materials and related systems for electronic, photonic and quantum device applications.

Abstracts

Twelve talks and sixteen posters, with the page number of each abstract. Talks are in programme order; posters are ordered by presenting author.

TALKS

T1	Anirban Das	28
	<i>Spin-orbit interaction and g-tensor anisotropy of holes in nanowires of hexagonal germanium</i>	
T2	Guido Wiersma	30
	<i>Electronic characterisation of hex-SiGe/Si core/shell nanowires</i>	
T3	Enrico Degan	31
	<i>Non-linear optical spectroscopy of hexagonal SiGe alloys</i>	
T4	Perpetua Muchiri	33
	<i>DFT-1/2 study of the effects of intrinsic defects on the electronic structure of silicon polytypes</i>	
T5	Veronica Regazzoni	34
	<i>Structural defects in planar hexagonal Ge: from HR-TEM observations to atomistic simulations</i>	
T6	Giovanni Isella	36
	<i>Deposition of planar 2H-Ge on CdS by low-energy plasma-enhanced CVD</i>	
T7	Alexandre Courac	38
	<i>Hexagonal Si polytype 6H by in situ synthesis</i>	
T8	Denny Lamon	39
	<i>Branched nanowires for quantum dots and core-shell structures</i>	
T9	Santhanu Panikar Ramanandan	41
	<i>Planar epitaxy of direct band gap hexagonal germanium layers</i>	

T10	Fabrizio Rovaris	42
	<i>Role of the metastable Si-XIII structure in the diamond-to-hexagonal phase transition</i>	
T11	Mette Schouten	44
	<i>Growth kinetics of hex-SiGe on wz-GaAs core nanowires</i>	
T12	Yetkin Pulcu	45
	<i>Structural, electronic and optical properties of hexagonal GeSn from density functional theory</i>	

POSTERS

P1	Andrea Besana <i>Growth of planar hexagonal germanium enabled by LEPECVD</i>	48
P2	Patrick Del Vecchio <i>Tailoring spin–orbit interaction in Ge heterostructures for quantum devices</i>	50
P3	Aamir Ejaz <i>RHEED-assisted crystal phase engineering of GaAs nanowires as template for hexagonal SiGe</i>	52
P4	Riccardo Farina <i>Experimental determination of Auger recombination in hexagonal SiGe nanowires</i>	54
P5	Jonathan J. Finley <i>Pick-and-place nanowire integration into silicon photonic structures</i>	56
P6	Max Gerin <i>High-pressure study of hexagonal Ge grown by molecular beam epitaxy on self-assisted GaAs nanowires</i>	58
P7	Tim Goedkoop <i>Epitaxy of CdZnS buffer layers for the growth of planar hex-SiGe</i>	60
P8	Romaly Grijpma <i>Quantum dots in hexagonal GeSi nanowires</i>	61
P9	Marvin M. Jansen-Zilles <i>Growth of hexagonal germanium quantum rings</i>	63
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P11	Órla N. McElhatton <i>The nature of the band gap of wz-GaAs: temperature-dependent band structure and optical emission</i>	66
P12	Steffen Meder <i>Room temperature lasing from individual InAs nanowires</i>	68
P13	Antonio M. Mio <i>TEM analysis of textured silicon polymorph crystals obtained via nanoindentation and annealing</i>	70
P14	Reyhaneh Ramezani <i>Germanium–tin thin films and nanostructures for sustainable group-IV photonics</i>	71

P15	Charles Renard	73
	<i>Ga-induced cation exchange on m-plane CdS surfaces: towards wurtzite GaAs epitaxy</i>	
P16	Laetitia Vincent	75
	<i>Opportunities and challenges of epitaxy of metastable hexagonal semiconductors on m-plane surfaces</i>	

Posters can go up during the Monday morning coffee break and are taken down in the Tuesday morning break. The poster session itself is on Monday from 12:15 to 14:00, together with lunch.

Talks

In programme order. The presenting author is set in **bold**.

Spin-orbit interaction and g -tensor anisotropy of holes in nanowires of hexagonal germanium

Anirban Das¹, Baksa Kolok^{1,2}, Daniel Varjas^{1,3} and András Pályi^{1,2}

¹Department of Theoretical Physics, Budapest University of Technology and Economics, Hungary

²HUN-REN-BME-BCE Quantum Technology Research Group, Budapest, Hungary ³IFW Dresden and Würzburg-Dresden Cluster of Excellence ct.qmat, Germany

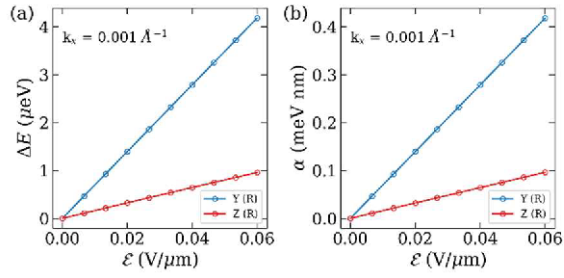
Hexagonal germanium (2H-Ge) offers strong spin-orbit interaction and optical activity, making it an appealing platform for semiconductor spin qubits. Recent progress in growing hexagonal $\text{Si}_x\text{Ge}_{1-x}$ nanowires enables controlled geometries suitable for quantum devices [1]. In contrast to cubic Si or Ge, 2H-Ge supports direct band-gap transitions, opening a pathway towards a novel spin-photon interface.

We study the electronic and spin properties of 2H-Ge nanowires using a multiband $k \cdot p$ Hamiltonian describing low-energy states near the Γ point [2]. We focus on nanowires oriented perpendicular to the c -axis and compute their band structure. We study the influence of transverse electric fields and extract the corresponding Rashba coefficients. We find that the strength of the Rashba effect depends strongly on the electric-field direction: for a y -directional electric field the Rashba strength ($6967 \text{ meV nm}^2/\text{V}$) can exceed that of other strong spin-orbit semiconductors over the same nanowire cross-section range, for example InSb ($400 \text{ meV nm}^2/\text{V}$). We also identify a strong confinement-induced renormalisation of the g -factor.

These results are essential for the development of semiconductor spin qubits and spin-photon interfaces based on quantum dots in hexagonal germanium.

REFERENCES

1. D. Lamon *et al.*, *Nano Lett.* **25**, 5741–5746 (2025).
2. Y. Pulcu *et al.*, *Phys. Rev. B* **109**, 245201 (2024).



(a) Rashba splitting and (b) Rashba coefficient as a function of electric field for two transverse directions of the nanowire.

Electronic characterisation of hex-SiGe/Si core/shell nanowires

G. Wiersma¹, R. E. Grijpma¹, R. Meijers¹, C. S. A. Müller¹, E. J. M. van de Logt¹, D. Lamon², M. M. Jansen², J. Ridderbos¹, E. P. A. M. Bakkers² and F. A. Zwanenburg¹

¹University of Twente, Drienerlolaan 5, 7522 NB Enschede, The Netherlands ²Eindhoven University of Technology, Groene Loper 3, 5612 AE Eindhoven, The Netherlands

As the need for more computational power increases, new platforms are being investigated in parallel with the further optimisation of standardised ones. One of those new platforms is hexagonal silicon–germanium (hex-SiGe): the hexagonal (2H) crystal structure results in a direct-band-gap semiconductor, so hex-SiGe is an optically active material, allowing optical components to be integrated into conventional CMOS chips. In addition, hex-SiGe can host spin qubits, offering a new material platform for quantum computing [1–3].

Here we present measurements on hex-SiGe/Si core/shell nanowires, with the aim of characterising the material properties. Adding a Si shell enhances the electronic properties of hex-SiGe through the formation of a two-dimensional hole gas at the interface. We fabricate nanowire field-effect transistor devices and find that the transport properties vary along the length of the nanowire, indicating position-dependent material characteristics. We also find that the hole mobility of core/shell nanowires increases by approximately an order of magnitude compared with core-only nanowires.

These measurements increase our understanding of this novel material platform and can be used to fabricate quantum dot devices reliably, the first step towards optically addressable spin qubits in hexagonal germanium–silicon [4–6].

REFERENCES

1. C. Rödl *et al.*, *Phys. Rev. Materials* **3**, 034602 (2019).
2. E. M. T. Fadaly *et al.*, *Nature* **580**, 205–209 (2020).
3. D. Lamon *et al.*, *Nano Lett.* **25**, 5741–5746 (2025).
4. S. Conesa-Boj *et al.*, *Nano Lett.* **17**, 2259–2264 (2017).
5. F. N. M. Froning *et al.*, *Appl. Phys. Lett.* **113**, 073102 (2018).
6. M. Brauns *et al.*, *Appl. Phys. Lett.* **109**, 143113 (2016).

Non-linear optical spectroscopy of hexagonal SiGe alloys

J. Zöllner¹, **E. Degan**¹, S. Meder¹, M. F. Schouten², M. Jansen², E. P. A. M. Bakkers² and J. J. Finley¹

¹Walter Schottky Institut, TUM School of Natural Sciences, Am Coulombwall 4, 85748 Garching, Germany

²Department of Applied Physics, TU Eindhoven, Groene Loper 19, 5612 AP Eindhoven, The Netherlands

Group-IV semiconductors in the hexagonal lonsdaleite phase have recently emerged as a promising platform for silicon-compatible optoelectronics, owing to their fundamental direct gap in Ge-rich $\text{Si}_{1-x}\text{Ge}_x$ alloys, continuously tunable across the short-wave infrared [1]. The joint optical density of states near the Γ -point gap and its evolution with alloy composition remain only partially resolved, however, since linear absorption experiments are hampered by the nanoscale dimensions of the available samples. Despite the centrosymmetric nature of the $P6_3/mmc$ lonsdaleite structure, non-linear optical techniques provide additional access to the electronic structure and crystal symmetry through the alloy fluctuations that break that symmetry. Excitation in the mid-infrared combined with second-harmonic detection in the near-infrared also allows the use of highly sensitive Si-based detectors, and measurement at room temperature.

Here we demonstrate frequency-dependent second-harmonic generation (SHG) measurements on hex-SiGe nanowires of varying alloy composition, which enables resonant probing of the electronic band structure [3], while polarisation-resolved SHG gives direct access to crystal symmetries [4]. The experiments used a pulsed femtosecond OPO laser providing signal excitation from 1.1 to 1.6 μm and idler excitation from 1.7 to 4.0 μm , with pulse durations of approximately 200 fs. We observe a clear onset of the SHG response at energies corresponding to the band gaps of the respective hex-SiGe compositions when tuning across the one-photon resonance. Measurements on the GaAs nanowire core reveal a distinct two-photon resonance at higher energies, demonstrating that the low-energy SHG onset originates from the hex-SiGe shell. Polarisation-resolved SHG measurements further reveal a frequency-dependent rotation of the SHG lobes relative to the nanowire axis, indicating that the response is governed not only by nanowire geometry but also by intrinsic electronic properties related to the optical transition matrix elements.

Our results establish SHG spectroscopy as a powerful tool for probing band structure, crystal symmetry and oscillator strengths in hexagonal SiGe nanowires, opening a pathway towards comprehensive non-linear optical characterisation of emerging group-IV photonic materials.

REFERENCES

1. E. M. T. Fadaly *et al.*, *Nature* **580**, 205–209 (2020).
2. P. Borlido *et al.*, *Phys. Rev. Materials* **5**, 114604 (2021).
3. A. Shree *et al.*, *Nat. Commun.* **12**, 6894 (2021).
4. Y. Yu *et al.*, *Nanotechnology* **28**, 395701 (2017).

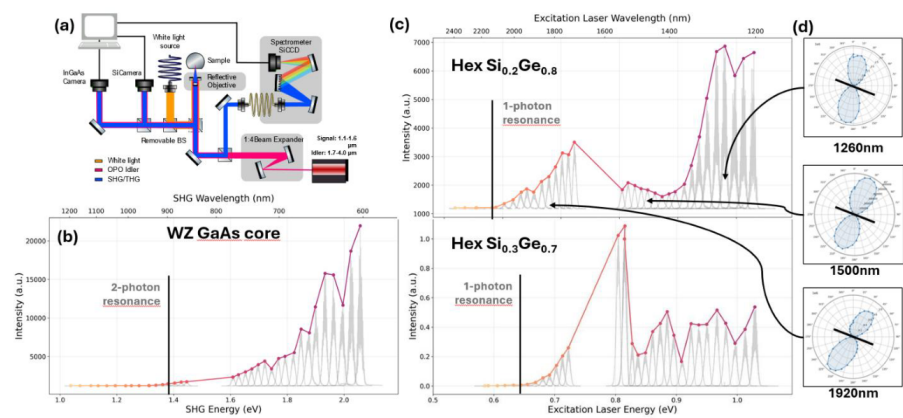


Figure 1. SHG response from Hex-SiGe alloys

DFT-1/2 study of the effects of intrinsic defects on the electronic structure of silicon polytypes

Perpetua Muchiri¹, Alberto Zobelli¹ and Michele Amato¹

¹Laboratoire de Physique des Solides, Université Paris-Saclay, CNRS, 91405 Orsay, France

Silicon is a key material for electronic, optoelectronic and photovoltaic applications, and its cubic diamond phase (3C-Si) has been studied extensively both experimentally and theoretically. Hexagonal silicon polytypes, including 2H-, 4H- and 6H-Si, have recently attracted growing interest because of their distinct structural and electronic properties [1–3]. Since these properties are strongly affected by intrinsic defects, an accurate description of band gaps and defect levels is essential. Conventional density functional theory (DFT) approaches such as the local density approximation (LDA) [4] and the generalised gradient approximation (GGA) [5] typically underestimate both.

To address these limitations while keeping the computational cost moderate, we employ the LDA-1/2 method [6], which efficiently corrects self-interaction errors and gives an improved description of semiconductor electronic structures. Using this approach we perform a first-principles investigation of the structural stability and electronic properties of silicon polytypes. Their relative stability is analysed through formation energies, and the electronic structure is characterised in terms of band gaps. We further investigate the effect of intrinsic vacancy-related defects, including monovacancies and divacancies.

Our results show that vacancy defects introduce localised states within or near the band gap, reducing the effective gap and modifying the electronic structure. Monovacancies mainly produce deep acceptor-like states, whereas divacancies generate a larger density of defect states because of stronger lattice relaxation. The defect-induced electronic response depends strongly on the crystal stacking sequence, with hexagonal polytypes showing greater sensitivity than cubic 3C-Si [7]. These findings give microscopic insight into defect physics in silicon polytypes and are relevant to the optimisation of silicon-based electronic and optoelectronic materials.

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Structural defects in planar hexagonal Ge: from HR-TEM observations to atomistic simulations

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Despite the significant challenges associated with stabilising germanium in its hexagonal (2H) phase, this material has recently attracted considerable attention as a promising platform for band-structure engineering and for next-generation electronic and optoelectronic devices. While 2H-Ge has so far been realised primarily in the form of core-shell nanowires, recent advances in the epitaxial growth of hexagonal Ge on CdS substrates have renewed interest in planar growth approaches and in the fundamental understanding of this metastable phase [1,2].

A major challenge arises from the lattice mismatch between the CdS substrate and the Ge epilayer, which induces elastic strain that relaxes through the nucleation of misfit and threading dislocations. At the same time, the intrinsic metastability of 2H-Ge favours local transitions towards the thermodynamically stable cubic (3C) phase, a behaviour already associated with specific dislocation configurations such as I₃-type defects in nanowire systems [3]. Dislocations therefore play a dual role, acting both as strain-relief mechanisms and as possible sources of cubic stacking insertions that degrade the structural quality of the hexagonal phase.

In this work we identify and classify the main dislocation types present in 2H-Ge/CdS heterostructures through a combined analysis of strain relaxation mechanisms and high-resolution transmission electron microscopy. We then construct atomistic models of the corresponding defect configurations, determining their slip systems and dislocation line orientations. The minimum-energy structures and their stability under finite temperature and applied strain are finally investigated through molecular dynamics simulations employing machine-learning interatomic potentials.

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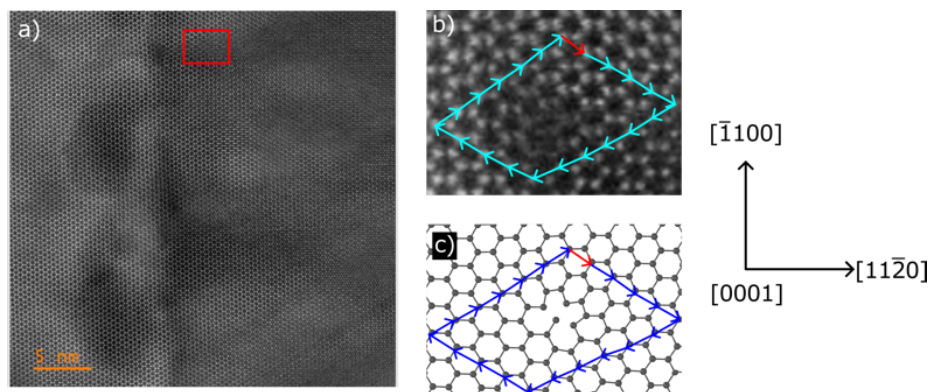


Fig. 1: Panel a: HR-TEM of 2H-Ge on Cds. Panel b: zoom of the red region in panel showing a dislocation. Panel c: atomistic model of the dislocation. The blue/cyan vectors represent the Burgers circuit, the red vector is the resulting Burgers vector.

Deposition of planar 2H-Ge on CdS by low-energy plasma-enhanced CVD

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Heteroepitaxy enables the use of quantum-confinement, band-gap and strain engineering to tailor precisely the electronic and optical properties of semiconductors. Controlling crystal symmetry has recently emerged as an additional and powerful way to tune the behaviour of group-IV materials. Notably, Ge can be synthesised in the hexagonal (2H) crystal structure, transforming it into a direct-band-gap semiconductor [1]. These results have been achieved by depositing 2H-Ge as a shell around a wurtzite GaAs core; the demonstration of planar 2H-Ge epilayers has so far met with only limited success [2].

We obtained planar 2H-Ge on CdS substrates using low-energy plasma-enhanced CVD, a growth technique well suited to low-temperature deposition. Consistent with previous reports, the temperature window for 2H-Ge nucleation is relatively narrow, with the best results obtained at approximately 250 °C. Transmission electron microscopy of 10 nm and 50 nm epilayers shows that the 10 nm layer has a predominantly hexagonal structure with a few inclusions featuring cubic stacking of the atomic planes. Molecular dynamics simulations employing machine-learning interatomic potentials suggest that these cubic domains form as a mechanism of strain relaxation. As growth proceeds the cubic fraction increases; from X-ray reciprocal-space maps we estimate a cubic fraction of approximately 30 %.

Both samples were characterised by photoluminescence spectroscopy, but none of the detected peaks could be unambiguously assigned to the epilayer, possibly because CdS exhibits several defect-related emission peaks in the short-wave infrared region [3].

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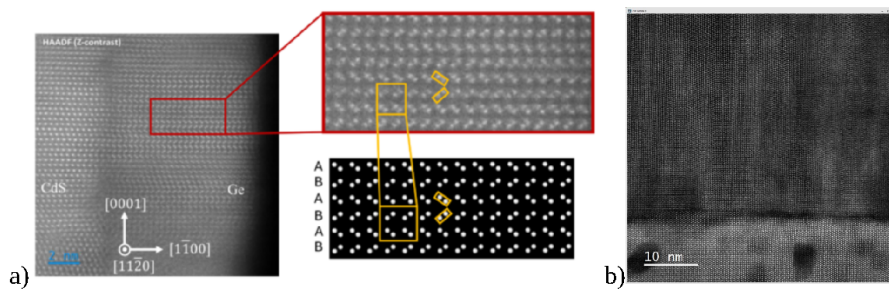


Figure 1 Comparison between a) a 10 nm and b) a 50 nm Ge layer deposited on CdS at 250°C.

Hexagonal Si polytype 6H by in situ synthesis

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The diversity of hexagonal forms of Si (Si-IV) can cover the surface of single-crystal diamond Si, Si-I [1], while most of them are absent from the equilibrium Si phase diagram [2] and are considered exotic metastable phases in bulk, if they exist at all. Most can be obtained using various large-volume high-pressure techniques [3]. In situ X-ray diffraction probing allows efficient and reliable synthesis both at high pressure (Paris–Edinburgh and various multi-anvil presses at synchrotron beamlines) and at pressures below atmospheric.

BC8 Si, or Si-III (body-centred cubic with eight atoms per unit cell), is a narrow-band-gap semiconductor [4] that crystallises well in high-pressure synthesis under quasi-hydrostatic conditions [5]. When heated, this phase produces a set of hexagonal Si phases, Si-IV. These are mostly polytypes of the diamond crystal structure: Si-4H, with a four-layer ABCB stacking sequence, differs from the equilibrium diamond structure with its three-layer ABC stacking (also denoted Si-3C).

Si-IV passes into Si-I at about 1273 K, and until very recently the mechanism of this transformation remained unclear. The diversity of possible hexagonal allotropes of Si derived from the diamond structure is in fact considerable. The frequently suggested Si-2H seems never to be observed in the high-temperature transformation of Si-III [6], and the hexagonal phase is nanostructured Si-4H. On heating, Si-4H passes into Si-6H, which is readily identified by in situ XRD and confirmed by Rietveld refinement [7]; this phase is nanostructured, like Si-4H.

In this presentation we discuss the prospects for optimising the synthesis of large-volume hexagonal Si, and the possibility of high-pressure phase transformation of hexagonal forms of Si–Ge solid solutions in large volume.

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Branched nanowires for quantum dots and core-shell structures

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Single-branched nanowires have proved a promising platform for realising hexagonal SiGe structures [1]. Compared with conventional core-shell nanowires they offer the key advantage of being separable from the GaAs core, giving a fully CMOS-compatible material system. They also provide access to a broader range of quantum properties than core-shell geometries, where confinement is limited to quantum wells [2]: branched nanowires enable both one-dimensional (quantum wires) and zero-dimensional (quantum dot) systems.

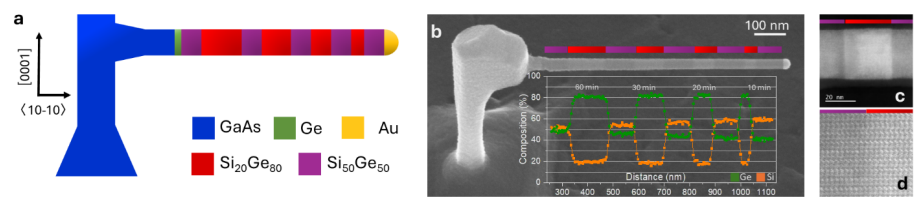
In this work we use the unique properties of branched nanowires to investigate the growth of hexagonal SiGe quantum dots with tunable size and composition, as well as core-shell nanowires free of III-V materials. We first demonstrate precise control over the Ge composition by adjusting the precursor gas ratios during growth, allowing each heterostructure segment to be defined accurately. The resulting quantum structures exhibit sharp, symmetric interfaces with widths below 5 nm, along with excellent tunability in both diameter and length. Full elastic relaxation is achieved at the heterointerfaces, ensuring defect-free material throughout the structure. Together these results enable precise control over the parameters governing quantum confinement, which is essential for high-quality quantum dots.

We then investigate the growth of Si and SiGe shells around these branches and quantum dots, for both surface passivation and strain engineering. A thin shell effectively reduces surface trap states, which are detrimental to optical and transport properties; thicker shells can instead introduce homogeneous strain, providing an additional degree of control over the electronic band structure.

Overall, branched nanowires appear as a versatile platform for engineering high-quality, CMOS-compatible quantum nanostructures of hexagonal SiGe, with finely tunable structural and electronic properties.

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Planar epitaxy of direct band gap hexagonal germanium layers

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Silicon and germanium are mainstream materials in modern electronics, but their indirect band gap limits their application in next-generation optoelectronic devices. In contrast, germanium and silicon–germanium alloys in the metastable hexagonal (2H) phase exhibit a direct band gap tunable across the mid-infrared range (1.8 to 3.5 μm) [1,2]. This material system has so far been realised only in the form of core–shell nanowires [1] and branched nanowire structures [3].

Here we demonstrate, for the first time, the planar epitaxial growth of hexagonal Ge (2H-Ge) layers on commercially available substrates. The key idea is to exploit a substrate with a hexagonal crystal structure to guide the atomic arrangement of the Ge layer during epitaxial growth. Using molecular beam epitaxy, 100 nm Ge layers are deposited on cadmium sulphide (CdS) and cadmium zinc sulphide ($\text{Cd}_{0.6}\text{Zn}_{0.4}\text{S}$)-buffered substrates. A systematic investigation examines how growth temperature and lattice mismatch influence hexagonal phase purity.

Structural and morphological analyses using atomic force microscopy, X-ray diffraction and transmission electron microscopy reveal that Ge layers grown on CdS exhibit mixed cubic and hexagonal phases. The hexagonal phase purity depends strongly on the growth temperature, with an optimum between 250 and 275 °C; at higher temperatures, thermochemical degradation of the CdS/Ge interface is observed [4]. Introducing a $\text{Cd}_{0.6}\text{Zn}_{0.4}\text{S}$ buffer layer brings two key benefits: it improves lattice matching with Ge, and it enhances the thermochemical stability of the CdZnS/Ge interface up to 350 °C, giving a marked increase in hexagonal phase purity.

Optical characterisation, including photoluminescence and absorbance measurements, is ongoing to confirm the direct-band-gap nature of the planar hex-Ge layers. Together these results establish a pathway for the planar integration of direct-band-gap group-IV semiconductors for mid-infrared photonics.

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Role of the metastable Si-XIII structure in the diamond-to-hexagonal phase transition

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Hexagonal diamond (hd) SiGe has recently been synthesised by exploiting core/shell nanowires, demonstrating a direct electronic band gap for Ge-rich hd-SiGe shells [1]. In the quest for a scalable way of synthesising such material, several possibilities have been proposed, among them the growth of SiGe films on planar wurtzite substrates [2] and the pressure-induced phase transition of a standard diamond cubic silicon wafer to hd by nanoindentation [3].

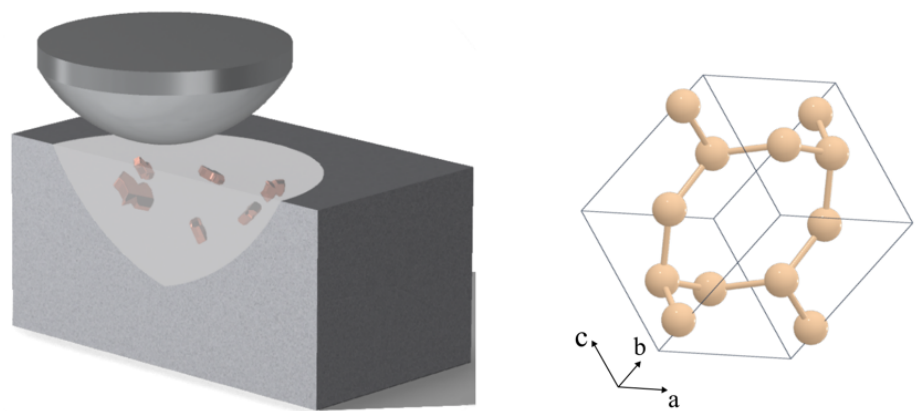
High-pressure experiments have revealed several metastable silicon allotropes along the transformation path from diamond cubic to hexagonal diamond. Among these, Si-XIII is particularly important and scientifically puzzling: first observed more than twenty years ago, this phase has remained structurally unidentified.

In this work we present a convergent methodology combining advanced theoretical modelling with experimental characterisation to resolve the long-standing structural assignment of Si-XIII [4]. We construct a structural model guided by experimental observations, validate it through first-principles optimisation, and systematically test it against multiple experimental signatures. All the key fingerprints of this phase (interplanar spacings, Raman frequencies, thermodynamic stability and kinetic pathways) are rationalised by our proposed crystal structure.

These findings provide a crucial missing piece in the high-pressure phase diagram of silicon, and a route to the monolithic integration of hd-SiGe on standard Si(001) wafers. The study further demonstrates the power of integrating computational predictions with experimental validation to resolve complex structural problems in materials science, opening new avenues for the controlled synthesis and functional exploitation of metastable group-IV allotropes.

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Growth kinetics of hex-SiGe on wz-GaAs core nanowires

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Novel approaches are required to integrate optically active components into silicon-based electronics. The group III–V semiconductors such as indium phosphide and indium gallium arsenide, currently used for these opto-electronic interconnects, have made great progress but remain scarce in nature. A more sustainable solution would be to develop a light source based on silicon itself, an approach hindered so far by silicon's indirect band gap.

An elegant way to adjust the band structure of Si is to organise it in the metastable hexagonal crystal phase rather than the naturally occurring cubic phase. Alloying hexagonal Si with hexagonal Ge gives a direct-band-gap material. To realise hex-SiGe, the periodicity of a wurtzite GaAs core nanowire is “copied” into a SiGe shell using metal-organic vapour-phase epitaxy (MOVPE). This core/shell system has proved suitable for tunable direct-band-gap photoluminescence emission [1], carrier confinement via quantum wells [2], and even amplified stimulated emission [3].

The high defect density is believed to affect the carrier dynamics in the hex-SiGe shell, which motivates an optimisation of the MOVPE growth parameters aimed at high crystal quality. We first investigate the growth dynamics near the GaAs–SiGe interface, showing that temperature plays a large role in the island morphology at the initial stages of SiGe shell growth. This island morphology can be linked to the nucleation of planar defects, enabling total suppression of planar defects at elevated growth temperatures. This enhanced material quality is not, however, reflected in an enhanced photoluminescence response: defects not distinguishable in transmission electron microscopy could be acting as non-radiative recombination centres. To control this defect density, homoepitaxy at larger shell diameters is evaluated, and two-temperature heterostructures are grown to isolate the impact of planar defects on the photoluminescence performance of the hex-SiGe nanowires.

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Structural, electronic and optical properties of hexagonal GeSn from density functional theory

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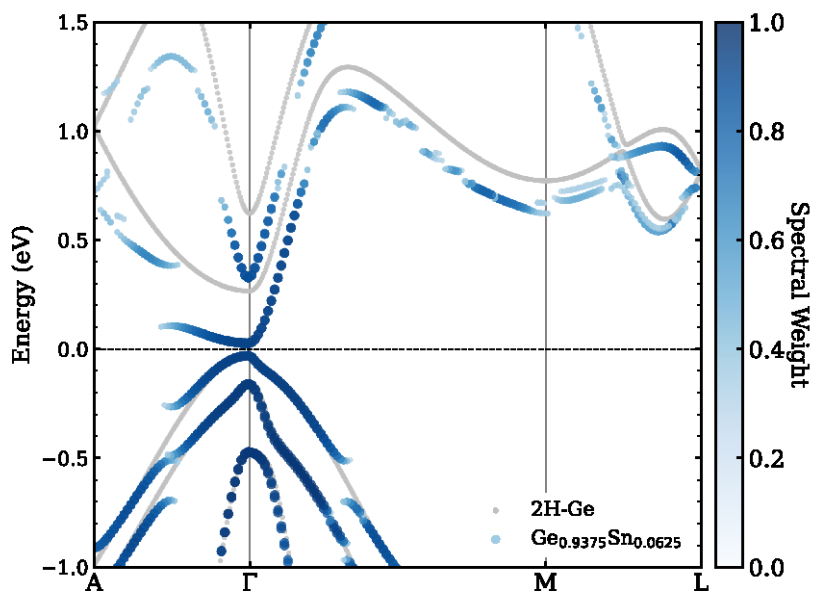
Unlike cubic GeSn, which requires a high Sn concentration to undergo an indirect-to-direct band-gap transition, lonsdaleite (2H) germanium is an intrinsic direct-gap semiconductor [1–3]. We employ first-principles density functional theory to investigate the structural, electronic and optical properties of 2H-Ge_{1-x}Sn_x random alloys [4,5] in the dilute Sn regime ($x \leq 0.10$). The extended alloy disorder is modelled using 48-atom special quasirandom structure supercells, and the coherent effective band structure is recovered via spectral band unfolding.

We show that 2H-Ge_{1-x}Sn_x maintains a direct band gap at the Γ point across the studied composition range, exhibiting a strong band-gap bowing that shifts the fundamental absorption edge into the mid-infrared. Evaluation of the optical transition matrix elements reveals a giant polarisation anisotropy dictated by spin–orbit coupling: the fundamental transition is strongly dipole-allowed for light polarised perpendicular to the crystal c -axis, an optical selection rule that is robustly preserved despite the random alloy disorder breaking the symmetry.

These results demonstrate that hexagonal GeSn bypasses the compositional threshold limitations of the cubic phase, providing a highly tunable direct-gap system for infrared optoelectronics.

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Posters

Presented during the poster session on Monday 14 September, 12:15–14:00. Ordered by presenting author, who is set in **bold**.

Growth of planar hexagonal germanium enabled by LEPECVD

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Germanium is a material of significant interest in semiconductor technology because of its electronic properties. The use of Ge, and of silicon, in optoelectronic devices nevertheless remains limited by the indirect band gap. Changing the crystal structure from the cubic phase to the metastable hexagonal phase gives hexagonal Ge (2H-Ge) a direct band gap. 2H-Ge has so far been grown mainly as core/shell nanowires [1], which inherently restrict the active volume; to overcome this constraint it is essential to synthesise high-quality planar 2H-Ge [2].

In this context we have grown 2H-Ge layers on wurtzite *m*-plane oriented cadmium sulphide (CdS) substrates by low-energy plasma-enhanced CVD, exploiting low-temperature epitaxy. Prior to the low-temperature growths on CdS substrates, a preliminary study of low-temperature epitaxy on Si substrates was conducted, yielding crystalline thin Ge epilayers even at ultra-low temperature.

The Ge/CdS samples were characterised structurally and optically by high-resolution X-ray diffraction (HR-XRD), energy-dispersive X-ray spectroscopy, high-resolution transmission electron microscopy (HR-TEM), Raman spectroscopy, photoluminescence and spectroscopic ellipsometry. Polarised Raman spectra of the 10 and 50 nm thick Ge/CdS samples show the transverse optical E_{2g} mode of 2H-Ge (about 288 cm^{-1} [3]), indicating the presence of the epitaxial crystalline 2H-Ge phase. HR-TEM confirms this directly, and also reveals that part of the Ge film eventually relaxes to the cubic phase (3C-Ge). HR-XRD measurements show Bragg peaks corresponding to both the hexagonal and the cubic phase, with a ratio of roughly 2:1 between 2H-Ge and 3C-Ge.

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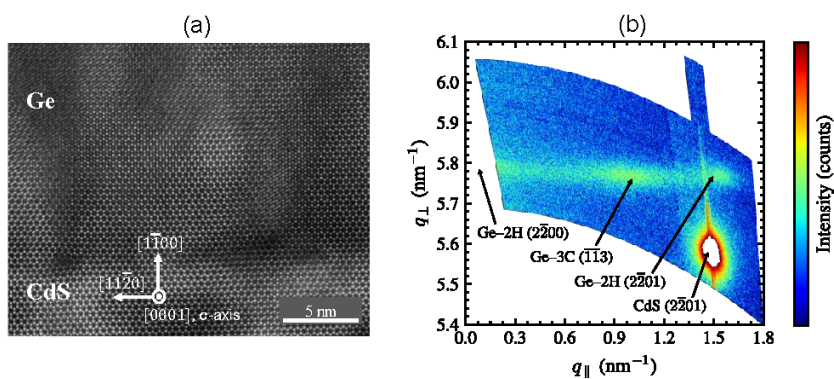


Fig. 1. (a) HR-TEM of the 50 nm-thick Ge/CdS sample. (b) HR-XRD reciprocal space map of the 50 nm-thick Ge/CdS sample around the CdS and Ge-2H($2\bar{2}01$) Bragg peaks.

Tailoring spin–orbit interaction in Ge heterostructures for quantum devices

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Quantum devices realised in planar Ge heterostructures benefit from strong intrinsic spin–orbit interaction (SOI), which enables efficient electrical control and engineering of the spin degree of freedom. The most advanced Ge/SiGe heterostructures to date, based on compressively strained Ge channels within strain-relaxed SiGe barriers, exhibit weak SOI because of the heavy-hole character of the wave function. This poses challenges for spin-based quantum devices and requires complex device designs for fast qubit manipulation.

In this work we demonstrate that concrete heterostructure modifications can overcome these limitations, enhancing SOI by up to three orders of magnitude [1]. Specifically, we propose to enrich unstrained Ge channels with localised, strained silicon spikes. Using multi-objective Bayesian optimisation, we optimise the spike profile to maximise SOI while ensuring compatibility with current epitaxial growth processes and robustness against realistic variations of growth parameters.

Our heterostructure substantially enhances device performance, yielding quantum-dot spin qubit quality factors up to two orders of magnitude higher than state-of-the-art materials. We also predict GHz-scale spin splittings for hybrid superconducting Andreev spin qubits. Ge heterostructures with engineered Si concentration profiles can open pathways to scalable quantum and spintronic applications.

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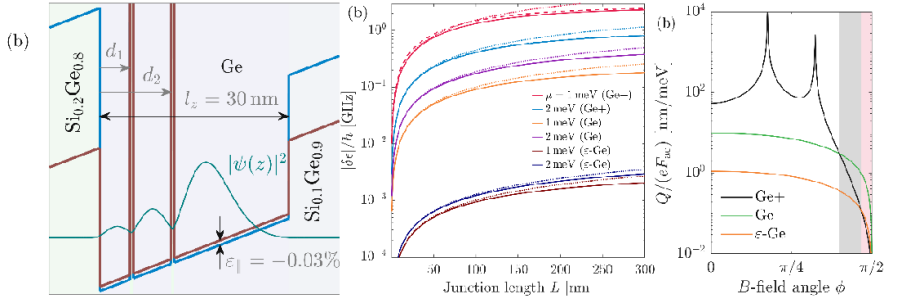


Figure : (left) Energy band alignment against the growth position of $\text{Ge}+$ with Si spikes. Optimization parameters are also shown. (Middle) Andreev Spin Qubit (ASQ) against junction length for various chemical potentials. Comparison between standard strained Ge , unstrained Ge and $\text{Ge}+$ with Si spikes. (right) Quality factor against the magnetic field in-plane angle with respect to the electrical driving axis.

RHEED-assisted crystal phase engineering of GaAs nanowires as template for hexagonal SiGe

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Silicon is the foundation of modern telecommunication technologies, but its indirect band gap limits its use as an efficient light source. Recent studies have shown that transforming SiGe from its conventional cubic structure into a hexagonal phase can induce direct-band-gap behaviour, opening new opportunities for silicon-compatible lasers and integrated photonic devices [1].

In this work we investigated the growth of self-assisted GaAs nanowire cores as crystal templates for a hexagonal SiGe (hex-SiGe) shell on silicon substrates. Achieving a phase-pure wurtzite (WZ) GaAs template is a critical requirement for the subsequent crystal phase transfer and epitaxial growth of the hex-SiGe shell, so precise control of the nanowire crystal structure during molecular beam epitaxy is essential. To that end we investigated the effect of As content on the GaAs WZ phase, and the effect of the ramping rate of As from low to higher content.

Reflection high-energy electron diffraction (RHEED) was employed as an in situ monitoring tool during nanowire growth, providing real-time information on surface structure, crystal quality and phase evolution through the symmetry and intensity of the diffraction pattern [2]. The technique enabled identification of the zinc blende and wurtzite crystal phases during growth, allowing growth conditions to be optimised for the desired WZ GaAs template.

The ability to monitor and control crystal phase in real time is a key step towards realising high-quality hex-SiGe heterostructures. Such structures offer significant potential for band-gap engineering through crystal phase design, quantum confinement, strain and doping, with the ultimate goal of developing silicon-compatible light sources for the telecommunication wavelength range (1.2–1.6 μm).

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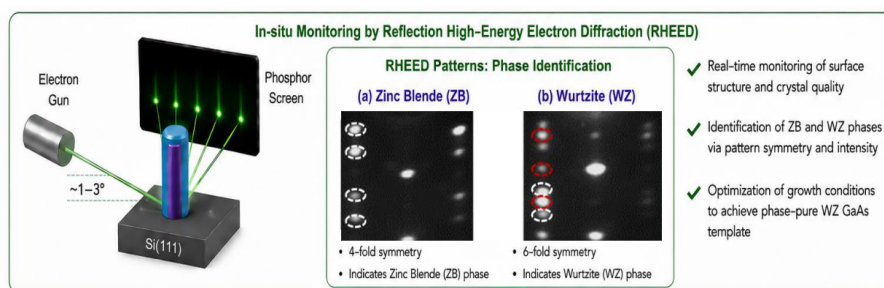


Fig. In situ Rheed monitoring of GaAs nanowires core as crystal template for SiGe shell.

Experimental determination of Auger recombination in hexagonal SiGe nanowires

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Hexagonal silicon–germanium (hex-SiGe) is a promising direct-band-gap semiconductor for silicon-integrated photonics [1]. Its narrow band gap raises concerns about high Auger recombination rates, however: this non-radiative process could severely degrade the efficiency of optoelectronic devices operating at high excitation, and hinder lasing [2,3].

Here we present the first experimental evidence of Auger recombination in hex-SiGe nanowires and assess its impact on optical performance. We extract the Auger coefficient from both continuous-wave and time-resolved photoluminescence data using an analytical model based on the rate equations. Excitation-dependent photoluminescence spectra show that the intensity increases according to a power law $I_{\text{PL}} \propto P^k$. At low excitation densities the slope $k \approx 1$, indicating the radiative limit; at higher densities k approaches 2/3, indicating the onset of Auger recombination. Time-resolved decay curves show carrier lifetimes dropping at higher powers, consistent with our model.

Across various nanowire geometries, growth patterns and germanium compositions (80 % to 100 %), the extracted average Auger coefficient is $(1.5 \pm 0.2) \times 10^{-29} \text{ cm}^6/\text{s}$. A systematic comparison with a broad range of other semiconductors demonstrates that the Auger recombination rate in hex-SiGe is comparable to, or up to an order of magnitude lower than, that of narrow direct-band-gap III–V materials such as InAs [4]. These results confirm that Auger recombination is sufficiently suppressed that it does not constitute a fundamental barrier to achieving lasing and to developing high-performance hex-SiGe photonic devices.

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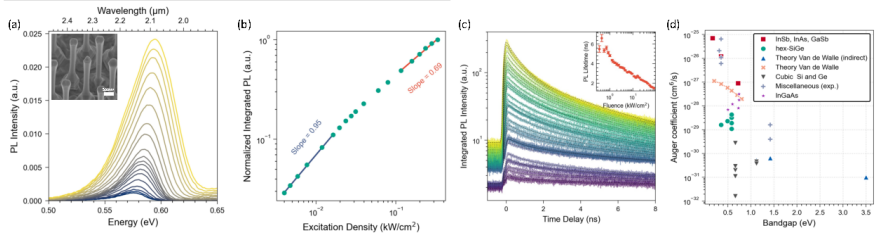


Figure 1: (a) Power-dependent PL spectra. Inset: 30° tilted SEM image of as-grown NWs. (b) Log-log LILO curve from integrated spectra in (a). Linear fits to the first (blue) and last (red) six points highlight the slope transition from ~ 1 (radiative) to $\sim 2/3$ (Auger). (c) TRPL decays at varying powers (integrated from 1350 to 2300 nm). Inset: Extracted effective PL lifetime vs. excitation power. (d) Auger coefficient vs. bandgap for hex-SiGe (green circles, varying Ge compositions) compared to other semiconductors. Colors/shapes denote distinct literature sources; InSb, InAs, and GaSb data were obtained using similar techniques [4].

Pick-and-place nanowire integration into silicon photonic structures

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Silicon photonic integrated circuits depend critically on compact on-chip light sources, for which nanowire lasers are an attractive solution. Their practical implementation is often limited, however, by broad emission linewidths and poor frequency stability resulting from weak optical feedback. Here we integrate individual nanowires by transfer printing into two types of silicon-on-insulator (SOI) cavity, to realise optical feedback at silicon-transparent wavelengths.

We first demonstrate transfer printing of individual hex-SiGe nanowires [1] into a photonic crystal (PhC) slot waveguide cavity [2] using a PDMS/PC approach. We then systematically investigate the self-localised resonant modes emerging from a comparable dielectrically loaded slot waveguide cavity, formed by introducing a Si segment in top-down fabrication. The resonance energy can be tuned from 0.465 to 0.61 eV, covering the full emission range of hex-Si_{0.2}Ge_{0.8}. Our findings indicate that the optical modes are determined predominantly by the photonic crystal geometry rather than the segment geometry, as evidenced by limited sensitivity to changes in segment length and position. For longer segments we observed higher-order PhC cavity modes and studied their spatial overlap with the segment.

We further integrate GaAsSb on silicon racetrack resonators by pick-and-place [3]. FDTD simulations reveal efficient coupling between the hybrid nanowire–waveguide mode and the fundamental TE resonator mode, with calculated cavity Q -factors exceeding 10^4 . Experimentally we observe feedback-induced lasing emission at a low threshold P_{th} of $8.6 \pm 1.8 \mu\text{J}/\text{cm}^2$. Compared with identical nanowire lasers without an SOI resonator, the linewidth is reduced by more than a factor of four at $3P_{\text{th}}$ and remains stable below 1.8 meV up to $5P_{\text{th}}$. Our results demonstrate nanowire-based light sources on SOI, and show that tailored resonator designs enable improved linewidth control and frequency stabilisation.

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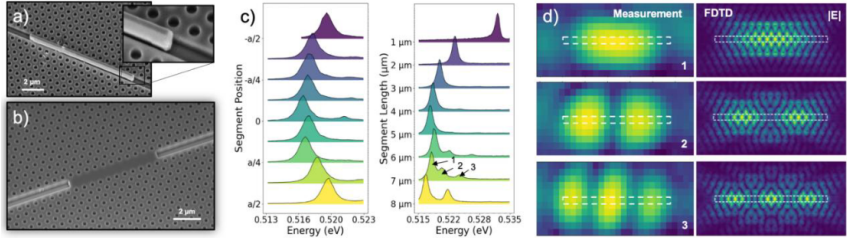


Figure 1. Integration of Hex-SiGe into a NW-induced PhC Cavity

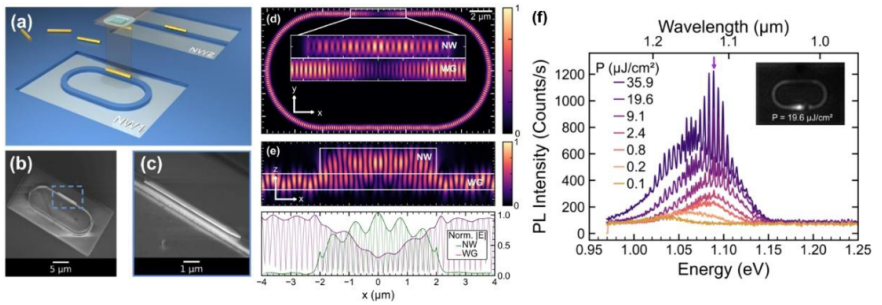


Figure 2. Lasing from SOI-integrated GaAsSb nanowires via resonator-driven optical feedback

High-pressure study of hexagonal Ge grown by molecular beam epitaxy on self-assisted GaAs nanowires

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Hexagonal group-IV semiconductors have attracted considerable attention because of electronic and optical properties distinct from those of the conventional cubic diamond phase [1]. Despite recent progress in growing metastable hexagonal (Si)Ge structures, their thermodynamic stability and structural evolution under compression remain poorly understood [2].

In this contribution we report an in situ synchrotron X-ray diffraction investigation of the high-pressure behaviour of hexagonal Ge nanowires grown by molecular beam epitaxy on GaAs nanowires [3]. Experiments were performed in diamond anvil cells up to 20 GPa at the ID27 beamline of the ESRF, under both hydrostatic and non-hydrostatic conditions.

A reversible transition from the semiconducting hexagonal phase to a high-pressure metallic phase was observed during compression, with the transition behaviour depending on the hydrostatic conditions. Under non-hydrostatic conditions the metallic phase does not revert directly to the hexagonal phase on decompression, but instead transforms into the metastable ST12-Ge phase, which is of interest for its potential for high-temperature superconductivity.

These results provide new insight into the stability of metastable hexagonal Ge and into the mechanisms governing pressure-induced structural transformations in hexagonal group-IV semiconductors.

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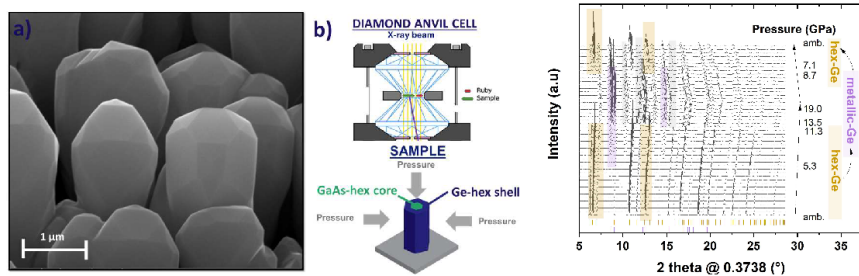


Figure. a) MEB image of GaAs@hex-Ge NW b) schematics of the diamond anvil cell experiment and nanowires c) X-ray diffraction pattern observed during pressure cycling

Epitaxy of CdZnS buffer layers for the growth of planar hex-SiGe

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Nanometre-scale regions of planar hex-Ge have recently been realised by molecular beam epitaxy on commercially available wurtzite CdS substrates, demonstrating that a hexagonal template can facilitate the planar formation of the metastable 2H crystal phase of Ge. The 2H phase purity has been found to be strongly limited, however, likely because of the large lattice mismatch of about 4 % and thermochemical degradation at the Ge/CdS interface. The latter has been shown to be reduced by the use of a ZnS layer. These results motivate the development of $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ buffer layers, in which Zn incorporation can simultaneously improve interface stability and tune the lattice parameters for a subsequent planar hex-SiGe layer [1].

In this work we investigate $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ buffer layers as tunable wurtzite templates for planar hex-SiGe epitaxy. The buffer layers are grown by molecular beam epitaxy on commercially available CdS substrates. The focus is on assessing the quality of the buffer layer, that is, its suitability for the subsequent epitaxy of planar hex-SiGe layers. Quality is evaluated on lattice matching to the targeted hex-SiGe composition, on surface morphology, and on crystal phase purity, specifically near the surface where the subsequent hex-SiGe epitaxy is initiated. The buffer layers are characterised using atomic force microscopy, X-ray diffraction and transmission electron microscopy.

We show that the lattice parameters of the buffer can be engineered by varying the Zn content. We also investigate the effect of the II/VI input flux on buffer layer quality, and compare $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ growth on *A*-plane and *M*-plane CdS substrates to assess the influence of substrate orientation.

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Quantum dots in hexagonal GeSi nanowires

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The CMOS industry is a highly developed industry working mainly with silicon and germanium. Because of their strong spin–orbit interaction, these materials are suitable hosts for spin qubits [1]. Large-scale quantum computation requires a large number of connected qubits [2]. Scaling problems could potentially be solved by forming a quantum internet, in which different quantum chips are connected using photons; and just as classical communication between computers is a vital part of modern technology, quantum communication between quantum devices would open new possibilities in quantum information science [3].

Our goal is therefore to couple spin qubits in a silicon or germanium platform with photons. In their standard cubic crystal structure these materials cannot be used efficiently for optical applications, as both silicon and germanium have an indirect band gap. This can be solved by growing a silicon–germanium alloy in the hexagonal (2H) crystal structure, referred to as hex-GeSi, which changes the band structure to a direct band gap [4]. Hex-GeSi can in this way be used to integrate optics into conventional silicon chips.

As this is a novel material, initial steps are needed before spin qubit devices that couple to light can be fabricated. Here we demonstrate the first measurements on quantum dot devices made from hex-GeSi nanowires grown at TU Eindhoven [5]. Bias spectroscopy measurements show clear and reproducible Coulomb diamonds. These measurements are the next step towards creating optically active spin qubits.

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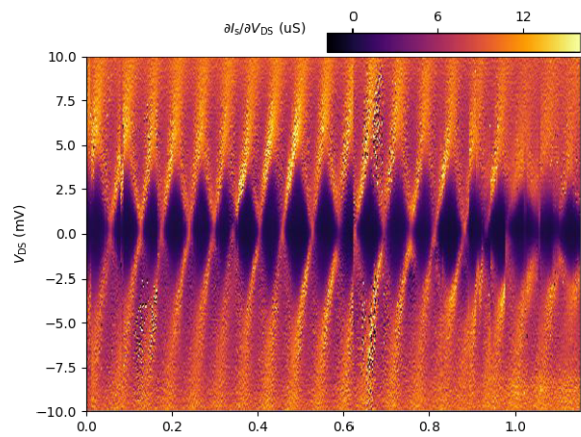


Figure 1 Bias spectroscopy measurement of a quantum dot in a hex-GeSi nanowire

Growth of hexagonal germanium quantum rings

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Hexagonal silicon–germanium (hex-SiGe) has emerged as a highly promising platform for scalable quantum information architectures [1,2], offering unique pathways to integrate optoelectronic properties with advanced quantum confinement. While type-I band alignment in hex-SiGe/Ge quantum wells highlights its potential [3], theory suggests that combining hexagonal and cubic Ge(Si) structures can further unlock precisely tailored electronic environments [4]. Enhanced flexibility in GaAs nanowire templates is now opening the door to silicon-based crystal-phase quantum wells [5].

Here we investigate the growth of hex-SiGe/Ge quantum wells on GaAs nanowires that alternate locally between wurtzite (WZ) and zinc blende (ZB) crystal phases, forming a ring-shaped hexagonal Ge segment. This quantum ring features dual confinement: crystal-phase-induced axial confinement, and radially controlled alloy composition.

We demonstrate that axial phase switching is achievable by briefly interrupting the arsenic supply during WZ growth, enriching the catalyst droplet with Ga to trigger a controlled WZ-to-ZB transition. The WZ/ZB superlattice growth mode in the GaAs nanowire template is supported by a vapour–liquid–solid growth model calibrated by TEM studies. Building on this, we achieve the growth of hexagonal/cubic SiGe alloys and Ge quantum wells embedded in SiGe shells, resulting in the formation of Ge quantum rings.

Our results introduce crystal-phase- and composition-modulated Ge quantum rings as a new platform for quantum information control in hex-SiGe.

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Defect engineering of SAE grown Ge nanowires for integrated photonics

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Germanium is a promising platform for CMOS-compatible integrated photonics, thanks to its compatibility with silicon technology and its optical response in the telecom wavelength range. In this work we investigate the selective area epitaxy (SAE) of Ge nanowires on Si substrates by metal-organic chemical vapour deposition, focusing on morphology control and defect engineering.

SAE consists of selectively growing Ge inside predefined openings patterned in a SiO₂ mask on Si substrates [1]. By tailoring the SAE geometry, Ge nanowires with widths ranging from 100 to 600 nm are obtained, corresponding to dimensions relevant for integrated photonic devices. Systematic variations of nanowire width and array pitch reveal pronounced changes in growth kinetics, morphology and faceting, highlighting the strong interplay between precursor diffusion, geometric confinement and loading effects during epitaxy. Distinct growth regimes emerge as a function of pitch and nanowire width, emphasising the importance of pattern design for achieving uniform, high-quality Ge nanowires.

Defect reduction and crystalline quality optimisation are investigated through flash lamp annealing (FLA), a rapid post-growth thermal treatment compatible with Ge nanowire integration. Recent studies on epitaxial Ge thin films have shown that FLA can significantly reduce threading dislocation density and provide insight into defect dynamics during thermal processing [2]. These results motivate the investigation of FLA in selectively grown Ge nanowires as a pathway towards improved crystalline quality and thermally induced strain control. X-ray diffraction, Raman spectroscopy and transmission electron microscopy are employed before and after FLA treatment to study crystalline quality and defect evolution.

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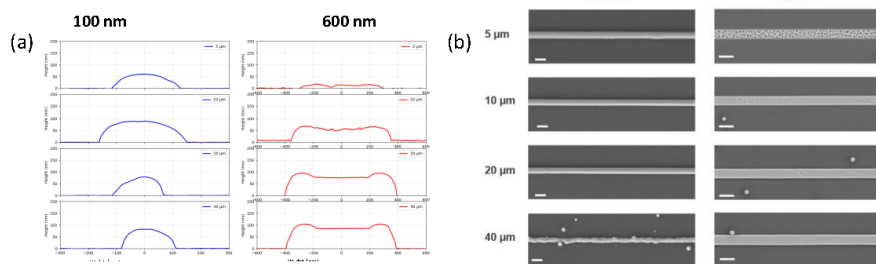


Fig. 1: (a) AFM line profiles extracted from nanowires with nominal widths of 100 nm and 600 nm with pitches ranging from 5 to 40 μm show a clear evolution of the cross-sectional shape and height distribution. (b) Corresponding SEM images confirming a strong dependence of morphology, surface roughness, and growth uniformity on pitch.

The nature of the band gap of wz-GaAs: temperature-dependent band structure and optical emission

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Conventional zinc blende GaAs (zb-GaAs) possesses a direct band gap and is widely applied in photonics. Metastable wurtzite GaAs (wz-GaAs), meanwhile, is employed for example as a template to facilitate the growth of lonsdaleite Ge nanowires, thanks to the low lattice mismatch [1]. In wz-GaAs the “pseudo-direct” Γ_{8c} conduction band state originates via back-folding of the L_{6c} conduction band edge state of zb-GaAs to the Γ point. At Γ , two conduction band states in wz-GaAs lie close in energy: the optically dark Γ_{8c} and the optically bright Γ_{7c} , the latter deriving from the direct zb-GaAs Γ_{6c} conduction band minimum.

The existing literature is inconclusive regarding the Γ_{8c} – Γ_{7c} ordering in wz-GaAs, that is, whether the band gap is pseudo-direct (dark) or direct (bright). Theory has generally predicted a pseudo-direct gap (Γ_{8c} minimum), while experimental interpretations have most often favoured a direct band gap (Γ_{7c} minimum) [2,3].

We address this discrepancy via systematic analysis of the temperature- and strain-dependent band structure of, and radiative recombination in, wz-GaAs, based on predictive density functional theory calculations. We show that DFT-calculated temperature-dependent optical transition energies agree quantitatively with experiment [3], but imply inverted Γ_{8c} – Γ_{7c} ordering compared with the previous experimental interpretation of the band structure [3]. We present a quantitative analysis of spontaneous emission [4] in wz-GaAs, and interpret the impact of strain via detailed comparison with experiment [2].

Our results quantitatively reassess the nature of the band gap, enhancing understanding of crystal-phase-engineered GaAs and guiding the engineering of novel and enhanced properties in semiconductor polytypes.

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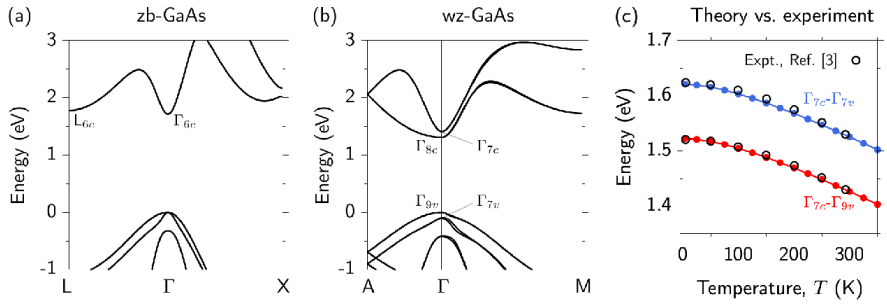


Fig. 1. DFT-calculated band structures of (a) zb-GaAs, and (b) wz-GaAs. (c) Theory (closed circles) vs. experiment (open circles) for the interband optical transition energies in wz-GaAs.

Room temperature lasing from individual InAs nanowires: a model system to compare with hexagonal SiGe

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Extending the emission wavelengths of monolithically integrated nanowire lasers to longer wavelengths, and even into the mid-infrared, shows great promise for optical on-chip communication and sensing applications using the mature silicon photonic circuit platform. Strong absorption within the visible range in silicon waveguides necessitates the integration of lasers emitting in the near- or mid-infrared for low-loss optical transmission. While examples of nanowire lasers have been shown with emission from the near [1] to the mid-infrared [2], few operate at the room temperature necessary for on-chip processors.

In this contribution we investigate the temperature-dependent lasing properties of InAs nanowires as a model system to compare with hexagonal SiGe nanowires. Individual nanowires are optically excited using pulsed excitation, and data are recorded as a function of lattice temperature. Finite-difference time-domain simulations give the diameter-dependent threshold gain for room- and low-temperature lasing emission from wurtzite-dominated InAs nanowires near 0.415 and 0.450 eV respectively.

To understand the modal contributions in the temperature-dependent lasing spectra, two sets of nanowires are chosen for micro photoluminescence measurements. For $D_{\text{NW1}} = 871 \pm 30$ nm, a dominant contribution of the TE_{01} mode is expected, as previously reported under continuous-wave excitation [3], while for $D_{\text{NW2}} = 1040 \pm 30$ nm multiple different axial modes are expected to have a low threshold gain. Spectra of the second nanowire above the lasing threshold, for temperatures ranging from 10 to 300 K, show multimodal lasing up to room temperature. Time-resolved measurements of the emission dynamics from individual InAs nanowires will also be presented.

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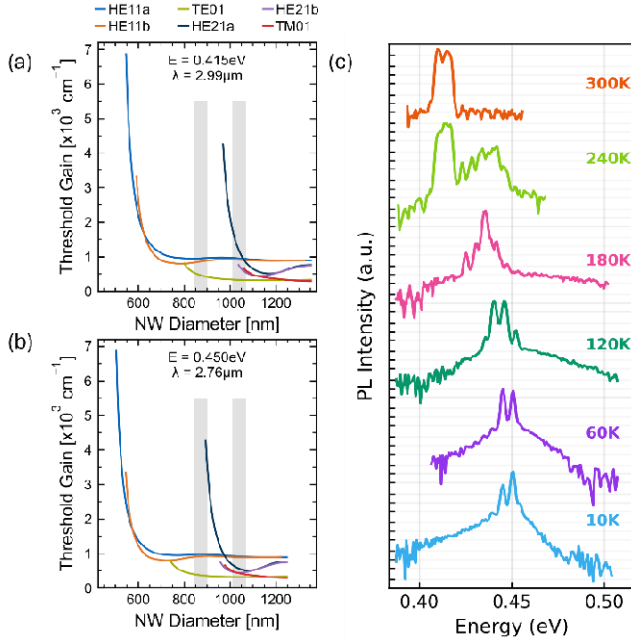


Figure 1: FDTD simulations of the threshold gain for different guided modes for room (a) and low (b) temperature emission of a $10 \mu\text{m}$ long InAs NW, (c) Temperature dependent micro-PL spectra recorded from an individual InAs nanowire laser up to room temperature

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 band gap. Among these, hexagonal diamond (hd) silicon is particularly attractive for its potential use as a template for the epitaxial growth of hexagonal SiGe alloys, which can maintain a tunable direct band gap across a broad compositional range.

We recently demonstrated the formation of micrometre-sized, textured hd-Si crystals through nanoindentation followed by rapid annealing at 250 °C [1]. This approach offers a simpler alternative to more complex syntheses, such as those involving nanowires or sophisticated deposition systems. Under high mechanical pressure, diamond cubic silicon (dc-Si) transforms into a metallic β -Sn phase; on pressure release, by optimising the nanoindentation unloading, we observed, via Raman spectroscopy, the formation of a mixed body-centred cubic (bc8) and rhombohedral (r8) phase.

In this study we investigate nanoindented dc-Si (001) pits prior to annealing, gaining deeper crystallographic insight into the intermediate metastable Si phases. The system was analysed using polarised Raman spectroscopy and transmission electron microscopy; TEM micrographs revealed extensive regions of r8/bc8 phases, well aligned with the substrate.

As an alternative to rapid annealing at 250 °C for producing hd-Si [1], we also explored the effects of other annealing processes at lower temperatures and rates, leading to the formation of other polymorphs such as Si-XIII, a metastable phase with a particular crystal structure that we recently resolved by convergent theory and experiment [2].

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Germanium–tin thin films and nanostructures for sustainable group-IV photonics

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$\text{Ge}_{1-x}\text{Sn}_x$ is a group-IV semiconductor with a band structure tunable into the telecommunication band by adjusting the Sn content. Unlike most III–V semiconductors, GeSn can be monolithically integrated on silicon while remaining CMOS compatible. Incorporating Sn into Ge lowers the direct Γ valley relative to the indirect L valley, enabling a transition towards a direct band gap with absorption and emission beyond 1550 nm [1]. The Sn content required for this transition depends strongly on strain, with GeSn on Si showing stronger strain relaxation than GeSn on Ge because of the larger lattice mismatch [2]. Understanding how strain and composition influence the optical properties of GeSn is therefore important for designing efficient group-IV infrared photonic devices.

In this work GeSn thin films are deposited by magnetron sputtering on both Ge and Si substrates. Reciprocal space mapping is used to determine the Sn content and strain state of the layers. GeSn on Ge is largely pseudomorphic up to about 8 at.% Sn, while GeSn on Si reaches about 12 at.% Sn and shows stronger strain relaxation. Optical properties are investigated using spectroscopic ellipsometry and Fourier-transform infrared (FTIR) spectroscopy. A parameterised semiconductor oscillator model [3] is used to extract the dielectric functions and interband transition energies, and FTIR with Tauc analysis is used to estimate indirect and direct band gaps. By comparing GeSn on Ge with GeSn on Si, this work aims to clarify the role of strain and Sn content in the indirect-to-direct band gap transition.

In parallel, post-growth annealing studies are performed to investigate crystalline quality and strain in group-IV materials. Flash lamp annealing (FLA) is being investigated on Ge/Si structures, where preliminary results show a reduced rocking curve full width at half maximum, indicating improved crystalline quality and the onset of partial or full melting [4]. This provides a basis for future studies of FLA on GeSn/Si for improving crystalline quality while preserving the metastable GeSn alloy.

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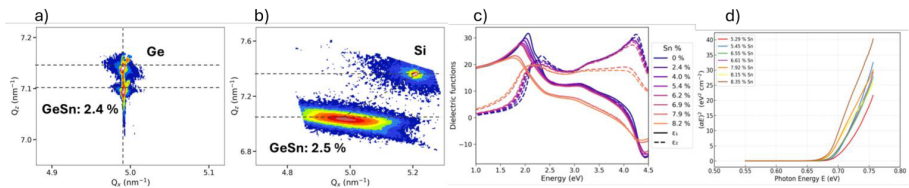


Fig. 1. RSM of the (224) reflection in $\text{Ge}_{1-x}\text{Sn}_x$ thin films on (a) Ge, (b) Si substrates, (c) Dielectric functions of $\text{Ge}_{1-x}\text{Sn}_x$ on Ge substrate, (d) direct bandgap energies of $\text{Ge}_{1-x}\text{Sn}_x$ as a function of Sn % for strained thin films on Ge substrate.

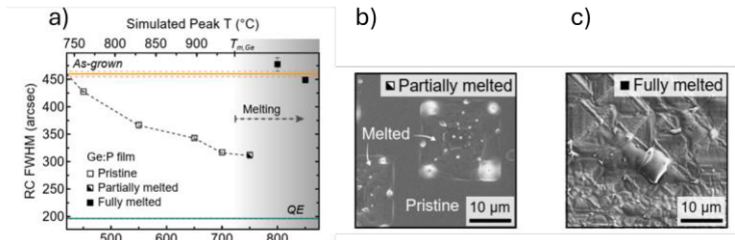


Fig. 2. Evolution of the XRD rocking curve FWHM of epitaxial Ge/Si after single-pulse flash lamp annealing (FLA) as a function of pre-heating temperature, showing improved crystalline quality and the onset of partial/full melting. SEM images show partially and fully melted Ge surfaces after FLA.

Ga-induced cation exchange on *m*-plane CdS surfaces: towards wurtzite GaAs epitaxy by vapour phase epitaxy

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The stabilisation of wurtzite GaAs remains a major challenge for III–V epitaxy, because the zinc blende phase is thermodynamically favoured in bulk materials. Hexagonal CdS substrates provide an attractive template for promoting metastable wurtzite GaAs, especially using non-polar *m*-plane orientations that favour hexagonal stacking propagation.

In this context we investigated the initial interaction between Ga precursors and *m*-plane CdS surfaces prior to GaAs growth by ultra-high-vacuum vapour phase epitaxy. During GaAs deposition using trimethylgallium (TMGa) and tertiarybutylarsine, we systematically observe the formation of an interfacial CdGaS ternary alloy before any detectable arsenic incorporation. Understanding this interfacial reaction is therefore essential for controlling the nucleation of wurtzite GaAs on CdS.

To elucidate the mechanisms involved, CdS surfaces were exposed solely to Ga precursors under various conditions. The influence of exposure time and precursor chemistry (TMGa versus triethylgallium) was investigated by in situ X-ray photoelectron spectroscopy, which reveals the progressive disappearance of Cd together with the formation of Ga–S bonds, indicating a Ga-for-Cd substitution process [1]. Cross-sectional STEM-HAADF and EDX analyses demonstrate the formation of a buried CdGaS alloy underneath a GaS-rich top layer, whose thickness and crystalline structure depend strongly on precursor chemistry and exposure duration. X-ray diffraction further confirms the epitaxial relationship between the transformed interfacial layers and the hexagonal substrate.

These results support a cation exchange mechanism assisted by the decomposition chemistry of organometallic precursors, particularly the methyl ligands of TMGa. Such interfacial reconstruction likely plays a key role in defining the structural template for subsequent wurtzite GaAs nucleation on *m*-plane CdS.

Beyond Ga precursors, preliminary experiments using trimethylaluminium indicate a strongly reduced diffusion of Al into CdS compared with Ga, suggesting that Al may remain confined near the surface instead of inducing deep cation exchange. This behaviour, likely related to the stronger Al–S bond [2], could enable improved interface abruptness and provide a promising route towards the stabilisation of hexagonal III–V heterostructures.

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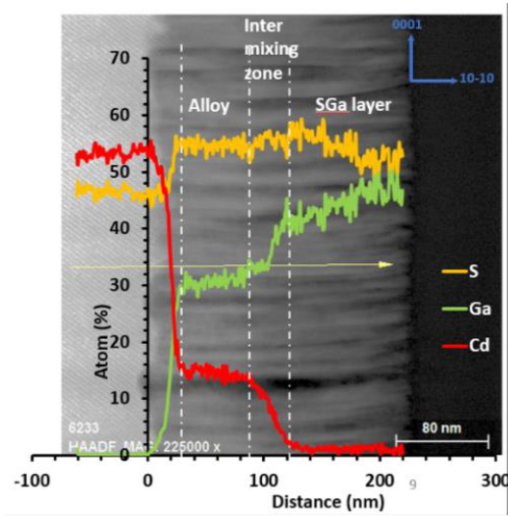


Figure 1. STEM-HAADF image with EDX profiles of a CdS substrate exposed during 15 min to TMGa precursor at 500°C

Opportunities and challenges of epitaxy of metastable hexagonal semiconductors on *m*-plane surfaces

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Crystal phase engineering, achieved through controlled modification of stacking sequences, is a promising strategy for tailoring material properties and enabling new functionalities. In particular, symmetry reduction in hexagonal polytypes alters the electronic band structure of semiconductors and induces anisotropy, opening new opportunities in photonics.

The methodology is based on hexagonal substrates with *m*-plane surfaces, which under suitable conditions promote the transfer of hexagonal structural order. Here we review the controlled epitaxy of metastable hexagonal semiconductors grown as thin films on *m*-plane bulk substrates by MOVPE.

We first investigate the growth of ZnCdS thin films, with particular focus on composition control and its impact on phase stability; this study demonstrates successful replication of the hexagonal stacking sequence of 2H-ZnCdS on 2H-CdS substrates. We then address the growth of GaAs hexagonal polytypes and identify the key parameters governing crystalline quality. While phase replication can be achieved on stabilised 4H-ZnS substrates, growth on CdS remains more challenging, because of interfacial diffusion and ion-exchange processes that hinder epitaxy and need to be limited and carefully controlled.

Thin-film growth enables standard electrical and optical characterisation, allowing a comprehensive investigation of material properties including band gap values, emission mechanisms and carrier dynamics. Owing to its non-centrosymmetric hexagonal structure, 4H-GaAs exhibits a strong second-order non-linear optical response ($\chi^{(2)}$) combined with intrinsic birefringence, making it a promising platform for enhanced second-harmonic generation. Finally, hexagonal GaAs layers can serve as a template for the growth of SiGe thin films or vertical hexagonal nanowires showing light emission.

Altogether, this work establishes crystal phase engineering as a versatile and scalable route to designing semiconductor platforms that combine direct band gap emission with non-linear optical properties, paving the way towards integrated photonic and quantum devices based on metastable hexagonal materials.

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