2nd International Workshop on Hexagonal SiGe and Related Materials

4-5 April 2024
U4-08

Topics

- **Growth of Hex-SiGe nanowires and planar films**
- **Characterization and modeling of structural, electronic and optical properties of Hex-SiGe**
- **Pressure-induced phase transitions: towards Hex-SiGe**
- **Towards Hex-SiGe-based devices**
- **III-Vs, II-VIs and related materials**

Invited Speakers

Erik Bakkers (Eindhoven University of Technology)
Christopher Broderick (Tyndall-University College Cork)
Verena Maier-Kiener (Montan Universität Leoben)
Laetitia Vincent (C2N - Université Paris-Saclay)
Silvana Botti (Ruhr Universität Bochum)
Silvia Pandolfi (IMPMC - Sorbonne Université)
Dan Buca (Forschungszentrum Jülich)

https://workshop-hexagonal-sige-2024.unimib.it/

The workshop is organized by Prof. Emilio Scalise, Prof. Leo Miglio, Dr. Anna Marzegalli and Dr. Fabrizio Rovaris from Department of Materials Science, University of Milano-Bicocca.

UNIVERSITÀ DEGLI STUDI DI MILANO BICOCCA
Ministero dell'Università e della Ricerca
Finanziato dall'Unione europea NextGenerationEU

2nd International Workshop on Hexagonal SiGe and Related Materials - Program

Thursday April 4th, Room U4-08, University of Milano-Bicocca

- 9:00 Welcome
- 9:15 Introduction - Emilio Scalise/Leo Miglio (Unimib)

Session A.1 (Chairperson: E.Scalise)

- 9:30 **INVITED - Erik Bakkers (TU/e)**

  Recent progress in hex-SiGe growth and optical properties

- 10:05 **Wouter Peeters**

  Quantum wells with a direct bandgap in hexagonal Silicon Germanium

- 10:25 **Marvin van Tilburg**

  Stimulated Emission Spectrum Observed from hex-SiGe Nanowires

- 10:45 **Iuliia Dudko**

  Telecom band light emission from confined hexagonal Ge grown on self-assisted GaAs NWs by MBE

11:05-11:20 Coffee break

Session A.2 (Chairperson: E. Bakkers)

- 11:20 **INVITED - Christopher Broderick (Tyndall-UCC)**

  Engineering direct-gap optical emission in hexagonal Ge

- 11:55 **Matte Schouten**

  Observation of carrier cooling in direct band gap hex-SiGe

- 12:15 **Baksa Kolok**

  Spin and charge relaxation in hexagonal germanium nanowire quantum dots due to phonons

- 12:35 **Frank Glas**

  Why is it so difficult to grow hexagonal diamond nanowires of group IV semiconductors

12:50-14:00 Lunch

Session A.3 (Chairperson: S. Pandolfi)

- 14:00 **INVITED - Verena Maier-Kiener (Unileoben)**

  From cryogenic to high temperature conditions – the wide range of advanced nanoindentation to study semiconductor materials

- 14:35 **Gerald Schaffar**

  Maximizing the Output of Metastable Crystalline Phases During Nanoindentation of Silicon and Germanium

- 14:55 **Emilio Scalise/Antonio Mio**

  Results and challenges in obtaining the hexagonal diamond Si phase by nanoindentation

15:15-15:30 Coffee break

Session A.4 (Chairperson: V. Maier)

- 15.30 **INVITED - Silvia Pandolfi (Sorbonne Université)**

  High pressure synthesis of nanostructured 4H hexagonal silicon polytype

- 16:05 **Theo van den Berg**

  2H Transformation in Nanofins and Determination of the Habit Plane

- 16:25 **Fabrizio Rovaris**

  Atomistic Mechanisms of dc-hd Phase Transition in Si Nanoindentation

16:45 Poster Session & Refreshment

19:30 Dinner

Friday April 5th, Room U4-08, University of Milano-Bicocca

Session B.1 (Chairperson: C. Broderick)

- 9:00 **INVITED - Laetitia Vincent (C2N - Paris Saclay)**

  Synthesis and structural defects of hexagonal SiGe: towards the epitaxy

- 9:35 **Pim van den Berg**

  Towards optically addressable CMOS compatible spin qubits

- 9:55 **Nicolas Forrer**

  Germanium/Silicon Core Shell Nanowires for Spin/Hole Qubits Fabricated by Chemical Vapour Deposition

- 10:15 **Isabelle Bollier**

Electrical Characterization of Hexagonal Silicon Germanium Nanowire

- 10:35 **Hassan Melhem**

  Growth of planar wurzite ZnS as a template for Hex-SiGe

10:55-11:10 Coffee break

Session B.2 (Chairperson: L. Vincent)

- 11:10 **INVITED - Dan Buca (Jülich)**

  Opportunities and challenges in Group IV

- 11:45 **Andrea Fantasia**

  A data-driven interatomic potential for exploring kinetics of phase transitions in Germanium

- 12:05 **Arianna Nigro**

  Growth and characterization of Ge/SiGe planar heterostructures for spin qubit applications

- 12:25 **Daniel Chrastina**

  Planar germanium quantum wells for hybrid semiconducting-superconducting quantum circuit

12:45-13:45 Lunch

Session B.3 (Chairperson: D. Buca)

- 13:45 **INVITED - Silvana Botti (RUB)**

  Tuning Electronic Properties of Hexagonal SiGe Quantum Wells

- 14:20 **Yetkin Pulcu**

  Multiband k · p theory for hexagonal germanium

- 14:40 **Marc Tunica**

  Ab initio modeling of n-type and p-type doping in hexagonal-diamond silicon

15:00 Closing remarks & discussion

Poster Session

- **D. Lamon**, M. M. Jansen, M. A. Verheijen, E.P.A.M. Bakkers
  Growth of hexagonal SiGe nano-branches
- **M.M. Jansen**, W.H.J. Peeters, M.A. Verheijen, E.P.A.M. Bakkers
  High aspect ratio wurtzite GaAs nanowires as a platform for hexagonal SiGe
- **S. Meder**, B. Haubmann, F. del Giudice, P. Schmiedeke, J. Zöllner, G. Koblmüller, J. J. Finley
  Infrared InAs nanowire lasers as a model system to compare with hexagonal-SiGe gain media
- **X. Wang**, J. Zöllner, D. Liu, S. Meder, W. Peeters, E.P.A.M. Bakkers, J. Haverkort, J. J. Finley
  Purcell-enhanced quantum emission using hex-SiGe NW-induced photonic crystal cavity
- **D. Liu**, X. Wang, J. Zöllner, S. Meder, W. Peeters, E.P.A.M. Bakkers, Jos Haverkort, J. J. Finley
  Towards Hanle effect measurements of electron and hole g-factors in hexagonal SiGe nanostructures
- **J. Zöllner**, S. Meder, W. Peeters, E.P.A.M. Bakkers, G. Koblmüller, J. J. Finley
  Simulation and Fabrication of a Hex-SiGe NW-induced Photonic Crystal Cavity in Silicon
- **H.A.J. van der Donk**, D. Lamon, M.M. Jansen, M.A. Verheijen, J.E.M. Haverkort, E.P.A.M. Bakkers
  Growth of branched wurtzite GaAs nanowire for Hybrid III-V/IV heterostructures
- **C. Wakelkamp**, R. Farina, W.H.J. Peeters, E.P.A.M. Bakkers, J.E.M. Haverkort
  Carrier Dynamics in Hex-SiGe Quantum Wells
- P. Hemme, **M. Verseils**, J.B. Brubach, P. Roy, C. Renard, L. Vincent
  Toward the formation of 2H Germanium by HPHT conditions with in-situ FIR probe
- **H. Ameziane**, H. Melhem, G. Patriarche, T. Van den Berg, G. Hallais, C. Renard, L. Travers, L. Vincent
  Growing SiGe nanowires with the hexagonal phase
- **R. Farina**, M.A.J. van Tilburg, V.T. van Lange, W.H.J. Peeters, S. Meder, M.M. Jansen, J.E.M. Haverkort, E.P.A.M. Bakkers
  Characterizing Optical Cavities in hex-SiGe Nanowires
- **V.T. v. Lange**, A. Dijkstra, E.M.T. Fadaly, W.H.J. Peeters, M.A.J. v. Tilburg, E.P.A.M. Bakkers, J.E.M. Haverkort
  Lifetime and Optical Matrix Element of Hexagonal Ge
- **R. Koolen**, M.A. Verheijen, E.P.A.M. Bakkers
  Virtual substrates for planar hex-Ge
- **G. Vanacore**
  Ultrafast Transmission Electron Microscopy (UTEM): a new tool for dynamic investigation of matter at combined fs-nm resolutions
- **E. Scalise,** A. Marzegalli, F. Montalenti
  2D Hexagonal inclusions in Silicon and Germanium
- **D. Lanzoni,** F. Rovaris, L. Martìn-Encinar, A. Fantasia, R. Bergamaschini, F. Montalenti
  Accelerating simulations of strained Ge surfaces evolution via Machine Learning

Quantum wells with a direct bandgap in hexagonal Silicon Germanium

Wouter H.J. Peeters,[1,*] Victor T. van Lange,[1,*] Abderrezak Belabbes,[2, 3,*] Max C. van Hemert,[1] Marvin Marco Jansen,[1] Riccardo Farina,[1] Marvin A.J. van Tilburg,[1] Marcel A. Verheijen,[1, 4] Silvana Botti,[3, 5] Friedhelm Bechstedt,[3] Jos. E.M. Haverkort,[1] and Erik P.A.M. Bakkers[1]

[1]*Department of Applied Physics, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands*

[2]*Department of Physics, Sultan Qaboos University, P.O. Box 123, Muscat, Oman*

[3]*Institut für Festkörpertheorie und -optik, Fiedrich-Schiller-Universität Jena, Jena, Germany*

[4]*Eurofins Materials Science Netherlands BV, 5656 AE Eindhoven, The Netherlands*

[5]*Faculty of Physics, Ruhr University Bochum, Universitätsstrase 150, D-44801 Bochum, Germany.*

*These authors contributed equally to this work

The demonstration of direct bandgap emission from Hex-SiGe alloys marked a milestone in the development of Group IV light sources. The realization of quantum heterostructures would constitute the next step, allowing the creation of advanced low-dimensional optoelectronic devices based on the SiGe system. For example, lasing thresholds can be reduced by using the modified density of states of quantum wells (QWs). Here, we show for the first time the realization of quantum wells with a direct bandgap in the hex-SiGe system. Photoluminescence experiments on hex-Ge/$Si_{0.2}Ge_{0.8}$ indicate a type-I band alignment, with light emission up to room temperature. The QW thickness is varied, allowing us to shift the emission energy through quantum confinement. Additionally, the growth kinetics of hex-Ge/ $Si_{0.2}Ge_{0.8}$ are studied, highlighting an unexpected growth rate increase for QWs in multi-quantum well (MQW) structures. The insights from the growth kinetics studies, in combination with the type-I alignment, pave the way towards novel MQW structures that were not possible with the SiGe system until now.

Stimulated Emission Spectrum Observed from hex-SiGe Nanowires

Marvin A.J. van Tilburg, Riccardo Farina, Victor T. van Lange, Wouter H.J. Peeters, Wouter H.J. Peeters, Marvin M. Jansen, Jonathan J. Finley, Jos. E.M. Haverkort, Erik. P.A.M. Bakkers

The integration of a laser onto the silicon photonics platform is considered vital for the further development of computing technologies[1]. A silicon (Si) based laser is however lacking, as the common cubic-Si and germanium (Ge) are indirect semiconductors. Recently it has been reported that hexagonal silicon-germanium (hex-SiGe) has both a direct bandgap and efficient light emission[2,3]. Here we show strong indications of stimulated emission in the amplified spontaneous emission (ASE) regime for single hex-SiGe nanowires (NWs). These single hex-$Si_{0.2}Ge_{0.8}$ NWs were investigated using micro-photoluminescence (PL) experiments, where we combined a single photon detector and a Fourier transform interferometer to measure both the spectral and temporal information at single photon sensitivities. This enables us to do single nanowire PL experiments in an emission regime up to 2300 nm. In Fig. 1a the emission spectrum of a single hex-$Si_{0.2}Ge_{0.8}$ NW is shown as a function of the excitation density. The spectrum is made up of a broad spontaneous emission spectrum with several cavity-mode resonances emerging on top. In Fig. 1b it can be observed that the resonance peak indicated by the blue dashed line has a superlinear dependency on the excitation density above a laser fluence of 180 μJ/cm^2, with an exponential term of $k = 2.25 \pm 0.27$, after which the PL intensity saturates. Furthermore, linewidth narrowing is observed as the full-width half maximum (FWHM) of the resonance peak (4.8 meV) is narrower than of the emission background (66 meV). The resonance peaks have a Free Spectral Range of 24 ± 4 meV, matching the expected longitudinal mode spacing of the TE01 mode in the nanowire. These observations all indicate stimulated emission from Fabry-Pérot modes and that we have reached the ASE regime with a hex-SiGe NW laser structure. Thus, we show lasing can be achieved in hex-SiGe with achievable improvements in material quality and cavity design.

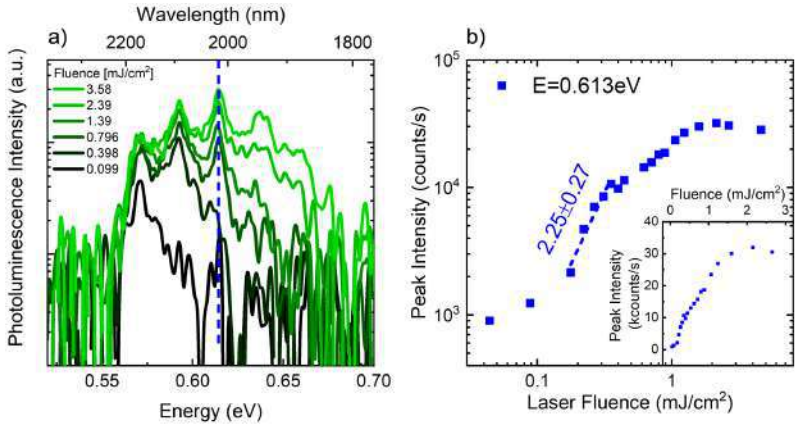


Figure 1 a) *Emission spectrum from a single hex-$Si_{0.2}Ge_{0.8}$ NW at different excitation densities on a logarithmic scale. The peaks have a free spectral range of 24±4 meV. The blue dashed line indicates the peak for which the intensity is given in Fig. 1b.* ***b)*** *Photoluminescence intensity of the peak at 0.613 eV as a function of the excitation density. The region of highest increase has been fitted by an exponential function, $I \propto P^k$ and shows a superlinear relation with $k = 2.25 \pm 0.27$. In the inset the intensity is given on a linear scale.*

1. Miller, D. A. B. Optical interconnects to silicon. *IEEE J. Sel. Top. Quantum Electron.* **6**, 1312–1317 (2000).

2. Fadaly, E. M. T. *et al.* Direct-bandgap emission from hexagonal Ge and SiGe alloys. *Nature* **580**, 205–209 (2020).

3. Van Tilburg, M. A. J. *et al.* Polarized emission from hexagonal-silicon-germanium nanowires. *J. Appl. Phys.* **133**, (2023).

Telecom band light emission from confined hexagonal Ge grown on self-assisted GaAs NWs by MBE

I. Dudko[a,b], A.D. Lamirand[a], C. Botella[a], P. Regreny[a], A. Danescu[a], M. Bugnet[c], M. Krämer[d], B. Gault[d,e], S. Walia[b], J. Penuelas[a] and N. Chauvin[a]

[a] *Ecole Centrale de Lyon, CNRS, INSA Lyon, Université Claude Bernard Lyon 1, CPE Lyon, INL, UMR 5270, 69130 Ecully, France*

[b] *School of Engineering, RMIT University, Melbourne 3001, Victoria, Australia.*

[c] *CNRS, INSA Lyon, Université Claude Bernard Lyon 1, MATEIS, UMR 5510, 69621 Villeurbanne, France.*

[d] *Max- Planck- Institut für Eisenforschung, Düsseldorf, Germany.*

[e] *Department of Materials, Royal School of Mines, Imperial College, London, UK.*

Corresponding Author: julia.dudko@ec-lyon.fr

In this work, hexagonal germanium (hex-Ge) was grown on the facets of self-assisted GaAs nanowires by MBE using VLS mechanism [1]. A pure wurtzite segment was maintained by adjusting the V/III ratio [2]. After growing the GaAs core, a Ge shell was grown with a long hexagonal segment. The crystal structure was characterized using high-resolution scanning transmission electron microscopy (STEM) to confirm the presence of hex-Ge.

We focused our investigations on the start of hex-Ge growth on GaAs nanowire facets. Measurements by atom probe tomography (APT) and STEM allow us to conclude that hex-Ge growth starts with the formation of small quantum dots (QDs) [Figure 1.a], which then expand until coalescing to form a radial quantum well. Photoluminescence (PL) spectroscopy performed on these hex-Ge/GaAs heterostructures shows a strong quantum confinement in these QDs leading to a light emission in the telecom bands. A redshift of the PL emission is observed when the QD size increases along with a strong decrease of the PL emission when the QD coalescence begins [Figure 1.b].

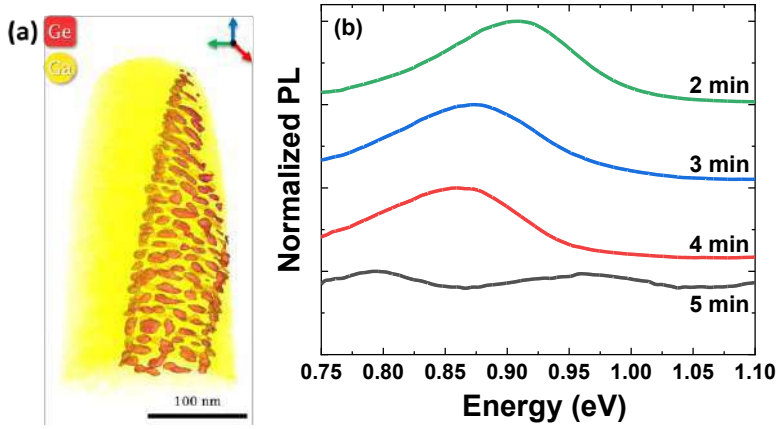


Figure 1: (a) APT showing small QDs. (b) low temperature PL as a function of the Ge growth duration in min.

[1] I. Dudko, Cryst. Growth Des. **22**, 32-36 (2022). [2] T. Dursap, Nanotechnology **32**, 155602 (2021).

Acknowledgments:
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).
We thank Uwe Tezins, Andreas Sturm, and Christian Broß for their support at the FIB & APT facilities at Max-Planck-Institut für Eisenforschung GmbH. M.K. and B.G. acknowledge financial support from the German Research Foundation (DFG) through DIP project no. 450800666.

INVITED

Engineering direct-gap optical emission in hexagonal Ge

Christopher A. Broderick[1,2,3,*]

[1]Tyndall National Institute, University College Cork, Lee Maltings, Dyke Parade, Cork T12 R5CP, Ireland
[2]School of Physics, University College Cork, Cork T12 YN60, Ireland
[3]Materials Department, University of California, Santa Barbara, California 93106, U.S.A.

*Email: christopher.broderick@ucc.ie

Experimental demonstration of direct-gap optical emission from Ge nanowires grown in the metastable lonsdaleite crystal structure ("2H-Ge") had heralded the emergence of a new candidate direct-gap group-IV semiconductor for applications in integrated Si photonics. However, the origin of this emission is puzzling from a theoretical perspective: analysis of the conduction and valence band (CB and VB) edge states indicates a forbidden transition, endowing 2H-Ge with a so-called "pseudo-direct" band gap.

I will begin by reviewing the theory of direct-gap optical emission in bulk 2H-Ge. I will demonstrate that first principles calculations of spontaneous emission (SE) spectra – based on density functional theory (DFT) – corroborate that observed photoluminescence (PL) from 2H-Ge nanowires is associated with radiative recombination across the direct fundamental band gap. Explicit DFT calculations show that the weak, but non-zero, zone-centre optical matrix element linking the CB and VB edges is governed by the spin-orbit interaction, confirming a recent group-theoretic prediction. Integrating the SE to compute the radiative recombination coefficient B reveals that it is approximately three orders of magnitude lower than in conventional direct-gap III-V semiconductors such as InAs. Strain-dependent calculations reveal, however, that the B coefficient at fixed temperature and carrier density can be increased by two orders of magnitude, suggesting that strain engineering of 2H-Ge is likely to be critical to enable laser applications. The analysis highlights that non-radiative recombination likely plays a dominant role in extant 2H-Ge nanowires.

Power-dependent PL measurements at low temperature have revealed the emergence of a secondary emission peak at high excitation intensity, lying approximately 40 meV above the primary band-to-band PL peak in energy. DFT calculations of the carrier density-dependent SE reproduce this behaviour. Detailed analysis highlights the key role of the wave vector dependence of the interband optical matrix elements in producing this secondary peak, and allow to predict the temperature dependence of this behaviour.

To provide a computationally inexpensive means by which to analyse the 2H-Ge optoelectronic properties, I describe the establishment and benchmarking of a 10-band **k.p** Hamiltonian for 2H-Ge, parametrised explicitly from hybrid functional DFT calculations. The truncation of the basis of bulk Bloch states employed as a basis to construct the Hamiltonian results, as described above, in a vanishing optical matrix element between the CB and VB edges. The conventional form of this Hamiltonian – which has been applied to hex-GaAs and 2H-Ge – thus precludes analysis of the optical properties. I describe incorporation of the pseudo-direct-gap optical matrix elements into the Hamiltonian. Using the eigenstates of the resulting **k.p** Hamiltonian to compute SE spectra allows to accurately reproduce DFT-based calculations, validating the model as a computationally inexpensive tool to analyse the optoelectronic properties of 2H-Ge.

Finally, I will present calculations of the electronic and optical properties of polytype heterostructures formed – along the crystallographic c-axis of the lonsdaleite structure – by alternating between the stable cubic (3C, ABC stacking) and metastable hexagonal (2H, AB stacking) crystal phases. DFT calculations confirm the presence of type-I band offsets in these heterostructures, with 2H-Ge/3C-Ge heterostructures forming an effective quantum well in which both electrons and holes are localised within 2H-Ge regions. Calculations as a function layer thickness demonstrate that (i) the formation of polytype heterostructures allows to tune the band gap across the application-rich 3 – 5 μm mid-infrared spectral range, and (ii) band hybridisation driven by interfacial symmetry breaking can, in short-period polytype superlattices, increase the band edge optical matrix element by up to an order of magnitude compared to its value in bulk 2H-Ge.

Observation of carrier cooling in direct band gap hex-SiGe

M.F. Schouten [a], M.A.J. van Tilburg [a], V.T. van Lange [a], W.H.J. Peeters [a], R. Farina [a], M.M. Jansen [a], M. Vettori [a], E.P.A.M. Bakkers [a], J.E.M. Haverkort [a]

[a] *Department of Applied Physics, Eindhoven University of Technology, Groene Loper 19, 5612AP Eindhoven, The Netherlands*

Efficient light emission and lasing require efficient carrier cooling towards the band edges by inelastic carrier-optical phonon scattering. The limited-to-non-existent Fröhlich interaction in group-IV materials implies that carrier relaxation should occur through deformation potential- or intervalley scattering. Further complications arise since the intravalley deformation potential scattering is forbidden near the Γ -point in s-like conduction bands. The high directness of hexagonal silicon germanium (hex-SiGe) opens the gate for experimental observation of carrier cooling in an isolated Γ-valley in a nonpolar semiconductor, which was hitherto not possible.

We measured the time-resolved photoluminescence (TRPL) spectra of hot carriers in hex-$Si_{0.2}Ge_{0.8}$ core-shell nanowires, as displayed in Fig 1a. The PL spectral line shape was fitted with a Lasher-Stern-Würfel (LSW) model, resulting in the carrier temperature as function of time ($T_C(t)$). Fig 1b displays the evolution of T_C with time. The initial carrier temperature is found to be dependent on the directness of the material. We interpret it to be a result of intervalley scattering from the bottom of the indirect minimum into the Γ-valley. The observed carrier cooling as a function of time is assigned to the remaining intravalley hot carrier cooling within the Γ-valley. The carrier relaxation is fitted using a mono-exponential decay function to extract a hot carrier lifetime (τ_0) of approximately 180 ps.

As expected, the intravalley carrier relaxation in the direct conduction band valley hex-SiGe is slower than in III-V semiconductors, which are dominated by the Fröhlich carrier optical phonon interaction. The hot carrier lifetime τ_0 of hex-SiGe is however found to be similar to a conventional InGaAs/InGaAsP MQW laser structure, which are known to be largely susceptible for the hot-phonon effect. This result shows that the nonpolar nature of our hex-SiGe nanowires does not provide a major obstacle for lasing.

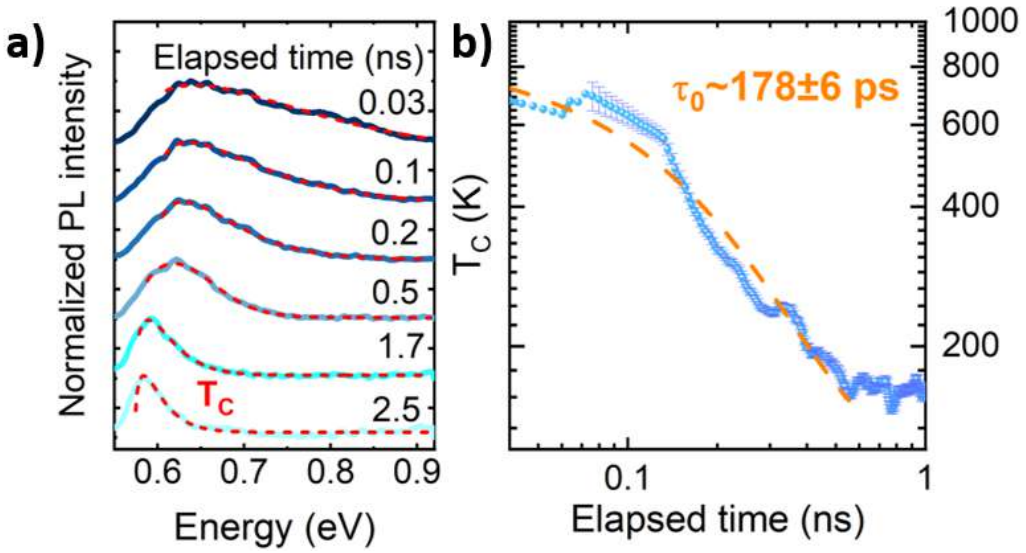


Figure 1: Carrier cooling in $hex-SiGe$. ***(a)*** *Waterfall plot of the normalized TRPL spectra as a function of time (dark to light) fitted with a LSW function (dashed red line) to extract the carrier temperature (T_C).* ***(b)*** *Carrier cooling curves fitted by a mono-exponential decay fit (dashed orange line) providing the hot carrier lifetime (τ_0).*

Spin and charge relaxation in hexagonal germanium nanowire quantum dots due to phonons

Baksa Kolok, György Frank, András Pályi
2024, Milan

Hexagonal germanium has a direct bandgap as DFT calculations and experiments show. The direct bandgap opens the way for optoelectronic applications of germanium and germanium-silicon alloys, which could represent important advances in conventional information technology and quantum information technology.

In our recent work, we studied the phonon dispersion relation in hexagonal germanium crystals. We started with the bulk crystal followed by the calculation of phonons in nanowires grown in the $[1\bar{1}00]$ crystallographic direction with square cross-section. We used linear elasticity theory to write up the equation of motion for acoustic phonons. We analyzed the modes with the COMSOL Multiphysics software numerically. For the lowest energy modes we used analytical approximations based on Landau and Lifschitz, and the results show agreement with high precision with the numerical data.

We have modeled the interaction between the spin qubits and the torsional phonon mode originating from the anisotropy of the material. This results in a direct coupling between the phonon mode and the spin-qubit through the g tensor. We have estimated the relaxation time coming from this interaction. We have also used the deformation potential formalism to model the electron-phonon interaction for the bending and longitudinal modes and estimated the charge relaxation times due to these phonon modes.This step is crucial to estimate the quality of the future spin qubits hosted in hex-Ge or hex-SiGe heterostructure.

Why is it so difficult to grow hexagonal diamond nanowires of group IV semiconductors?

Frank Glas
Université Paris-Saclay, CNRS, Centre de Nanosciences et de Nanotechnologies, Palaiseau, France

The hexagonal wurtzite (WZ) crystal structure is widely observed in nanowires (NWs) of III-V materials having a cubic zinc blende (ZB) bulk crystal structure, at least when they are grown in the vapor-liquid-solid (VLS) mode along the usual [111] direction. On the contrary, despite many attempts, the hexagonal diamond (HD) phase is rarely found in NWs of group IV semiconductors grown similarly. The aim of this short presentation is to ask why this is so, from the point of view of experiment-based growth models.

Our current understanding of WZ formation in NWs of compound semiconductors is largely based on two models and *in situ* TEM experiments. 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 ZB [1]. This requires that (1a) nucleation occurs at the triple phase line (TPL) bordering the interface, (1b) the *effective energy* of the nucleus 'facet' (1 ML high step) in contact with the vapor is lower for WZ than for ZB, (1c) the supersaturation of the liquid is high enough [1]. Condition (1a) has now been confirmed by *in situ* TEM [2,3] and (1b) is supported by *ab initio* calculations [4,5]. The second model is based on other *in situ* TEM results showing that, in a given NW, the WZ/ZB transitions correlate with changes of the NW/liquid interface morphology between planar and "truncated", occurring at critical values of the catalyst droplet contact angle β [6], with WZ only present at intermediate β, along with a planar interface. The model explains well how β determines the interface morphology, without however considering either nucleation or growth. Putting together the two models, it may be inferred that WZ growth is inhibited if the TPL disappears, which is the case if a truncation forms around the NW.

We will first discuss the processes at play in the III-V case and, in the light of published data and recent modeling [7], possible values of the relevant parameters (surface energies, supersaturation) in the case of GaAs. We will then briefly and cautiously examine which of the conditions (on geometry, crystallography, thermodynamics and growth conditions) found necessary for WZ formation might not be met for Si or Ge NWs, thereby preventing the standard growth of HD structures.

[1] F. Glas, G. Patriarche, J.-C. Harmand, Phys. Rev. Lett. **99**, 146101 (2007).
[2] J.-C. Harmand, G. Patriarche, F. Glas, F. Panciera, I. Florea, J.-L. Maurice, L. Travers, Y. Ollivier, Phys. Rev. Lett. **121**, 166101 (2018).
[3] M. Marnauza, M. Tornberg, E. K. Mårtensson, D. Jacobsson, K. A. Dick, Nanoscale Horiz. **8**, 291 (2023).
[4] R. Magri, M. Rosini, F. Casetta, Phys. Status Solidi C **7**, 374 (2010).
[5] V. Pankoke, P. Kratzer, S. Sakong, Phys. Rev. B **84**, 075455 (2011).
[6] D. Jacobsson, F. Panciera, J. Tersoff, M. C. Reuter, S. Lehmann, S. Hofmann, K. A. Dick, F. M. Ross, Nature **531**, 317 (2016).
[7] F. Glas, submitted to Phys. Rev. Mater.

Email: frank.glas@c2n.upsaclay.fr

Maximizing the Output of Metastable Crystalline Phases During Nanoindentation of Silicon and Germanium

Gerald J. K. Schaffar*, Verena Maier-Kiener
Department Materials Science, Montanuniversität Leoben, Roseggerstrasse 12, 8700 Leoben, Austria

*presenting and corresponding author: gerald.schaffar@unileoben.ac.at

It has been thoroughly investigated that indentation testing of loosely packed diamond-structure semiconductors causes phase transformations in these materials. These transformations lead either to the formation of amorphous material or the generation of metastable crystalline phases upon unloading. Thereby, the metastable crystalline phases are eagerly sought after, as they show electrically interesting properties and can be transformed into hexagonal phases upon annealing. Accordingly, to obtain more hexagonal material it is beneficial to tinker with the loading parameters during nanoindentation to create the maximum amount of metastable crystalline phases. The occurring phase transformations can be effectively tailored by varying both, the mechanical loading conditions and the testing temperatures.

In the case of silicon phase transformations occur up to 300 °C, whereas in the case of Germanium indentation temperatures should be kept below 0 °C. If these temperatures are surpassed the phase transformations will be suppressed in favor of dislocation plasticity in the diamond lattice. On the other hand, experimental temperatures should not be too low as then amorphous transformation rather than generation of metastable crystalline phases is favored. Accordingly, just below the onset temperatures for dislocation plasticity, a sweet spot for metastable crystalline transformation can be found. A further important consideration regarding mechanical loading is the choice of the tip geometry, as this also strongly influences the high-pressure phase transformations. Regarding loading parameters, slow unloading favors the formation of metastable crystalline over amorphous material. Even constant-load holding segments can be added to the unloading procedure to promote the generation of metastable crystalline material. Thereby the phase transformation can be influenced by the holding load and duration. In this presentation, a critical examination of these approaches will be shown and discussed regarding their applicability to the generation of metastable crystalline phases.

Results and challenges in obtaining the hexagonal diamond Si phase by nanoindentation

A. Marzegalli[1], A. Mio[2] , D. Spirito[3], F. Rovaris[1], M. Bikerouin [1], G. Shaffar[4], V. Meier[4], G. Capellini[3], E. Scalise[1]

1-L-NESS and Department of Material Science, Università degli Studi di Milano-Bicocca,Milano, Italy
2-CNR-IMM, Catania, ITALY
3-IHP GmbH, Innovations for High Performance Microelectronics, Frankfurt (Oder), Germany
4-Department of Material Science, Montanuniversität Leoben, Leoben, Austria

Exploiting the nanoindentation as an alternative approach to obtain the hexagonal diamond (hd) of Si will be discussed by presenting our recent results. Following a preliminary analysis of the optimal tip geometry and load aimed at obtaining the hexagonal diamond phase, we focus here on the results achieved by performing nanoindentation with spherical 10-20 μm indenter tips. Our extensive Raman analysis on all the pit arrays indicates that metastable BC8/R8 phases are always present after nanoindentation, using both indenter sizes.
Two different annealing approaches have been used to induce further transformation of the BC8/R8 metastable phases: stage annealing up to 220ºC and furnace annealing for two hours at ~255 ºC. The Raman analysis reveals that in both approaches the annealing induces the phase transformation of the BC8/R8 phases, whose Raman peaks completely disappear after annealing. However, the new Raman peaks are very different in the two cases.
With the stage annealing, Raman peaks compatible with the Si-XIII phase are clearly identifiable but evolve after aging (two weeks) at room temperature.
In the case of furnace annealing a dominant peak at around 520 cm^{-1} reappears but is accompanied by a broad shoulder centered at 513 cm^{-1}. In previous works, similar behavior of the Raman spectra was associated with the presence of the hexagonal phase.
The possibility of using polarized Raman spectroscopy combined with theoretical simulations to better identify the different metastable phases is also discussed.
Finally, a preliminary TEM/STEM analysis on one of the indentation pits after furnace annealing is also presented. Indeed, selected electron diffraction pattern (SADP) results are compatible with the presence of the hd phase. A more extended analysis including electron energy loss spectroscopy (EELS) is running to undoubtedly ascertain the transition to the hd phase.

Theo van den Berg, Geraldine Hallais, Charles Renard, Mette Schouten, Hassan Melhem, Hafssa Ameziane, Laetitia Vincent

Affiliation C2N – Paris Saclay

2H Transformation in Nanofins and Determination of the Habit Plane

We developed a process to partially transform both silicon and germanium from the cubic 3C phase to the hexagonal 2H phase. To initiate the transformation, HSQ is spinned around the nanostructures and cured to densify. Shear-induced stress and temperature are the main parameters for the transformation. We investigate the underlying processes and the mechanisms of transformation. By changing crystal orientation and geometry, the stress field is changed.

By producing an array of nanofins on (111) substrates with e-beam lithography, transformed domains are observed in the outer fins of the array. Different stress fields can be investigated according to the right parallelogrammic configuration. Two different shear stress situations are tested, one where mainly shear stress along the <110> direction is expected, and one with mainly <112> shear stress. For both configurations, TEM observations are carried out across the short side and the perpendicular one.

Along the cubic <110> zone axis, we observe several transformed 2H bands which display the <-2110>2H direction parallel to <1-10>3C . The bands are bounded by an interface of -5-7-5-7- membered rings of Si-atoms along a {115} plane.

However, when observing from the <112> zone axis (90° rotated) for the same stress configuration, the transformation observed from the <110> direction is not directly identifiable as 2H. Instead, a Moiré pattern can be observed. This transformed band can be highlighted with dark-field conditions. We confirmed that there are two different orientations of 2H domains in the nanofin and that the habit plane is the {115} plane and not inclined.

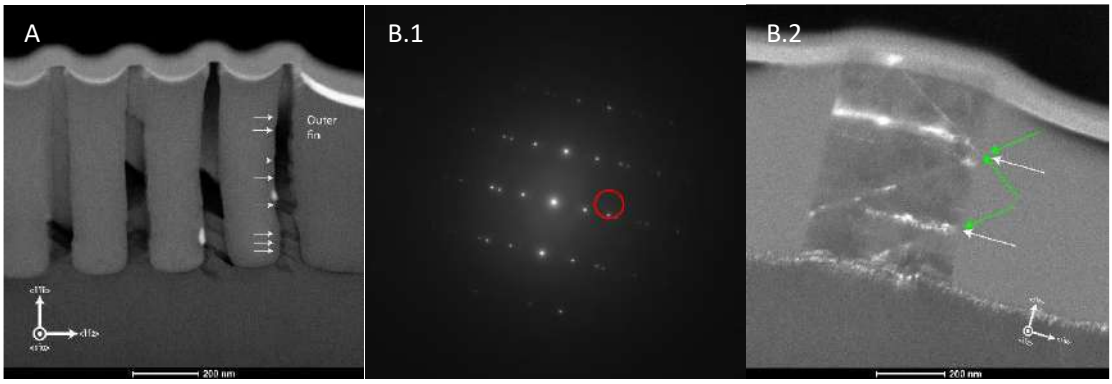


Figure 1 : (S)TEM images of two FIB cuts A and B made from the same sample with the same geometry and same stress fields respective to the crystal orientation. Most shear stress is expected along the <112> direction. In A, a BF-STEM image, the zone axis is <110> and the white arrows indicate confirmed 2H bands. The outer fin has more transformation than the inner fins. In B.1 electron diffraction pattern related to B.2. The red circle is where an aperture is placed to physically filter electrons. By putting the filter DF-TEM phases containing this specific diffraction spot are highlighted. This spot belongs to the 2H phase, and thus 2H is highlighted in B.2. The green arrows indicate confirmed 2H phases by changing to a <110> zone axis. The white arrows indicate vertical hidden 2H bands. More bands can be revealed by tilting the sample.

Towards optically addressable CMOS compatible spin qubits

P.D. van den Berg[1], C.S.A. Müller[1], D. Lamon[2], M.M. Jansen[2], A. Li[2],
J. Ridderbos[1], E.P.A.M. Bakkers[2] and F.A. Zwanenburg[1]
[1]University of Twente, The Netherlands
[2]Technical University Eindhoven, The Netherlands

The 2H hexagonal crystal phase of Si/Ge alloys (hex-GeSi) has recently shown to have a direct bandgap [1-3]. This material brings forward exciting photonic functionalities to the group IV semiconductors, such as a spin-photon interface and lasing, while being compatible with CMOS technology. Efficient light emission comparable to a direct bandgap group III-V semiconductor has been shown, with tunable photoluminescence spectra from 0.35 eV to 0.67 eV [3-4]. Hex-GeSi can be epitaxially grown in the form of nanowires, either in a core-shell or branch configuration. In this research, we perform electrical characterization of ultrathin hex-GeSi nanowire branches of diameters down to 10 nm. Together with our consortium partners, we are optimizing their transport properties, with the goal of forming electrostatically defined quantum dots. Following the approach used on high-quality cubic Si nanowires [5-7], we aim to develop optically addressable spin qubits in this CMOS compatible platform.

[1] C. Rödl et al., Phys. Rev. Materials, vol. 3, p. 034602, 2019.
[2] T. Kaewmaraya et al., The journal of Phys. Chem., vols. C121-10, p. 5820, 2017.
[3] E.M.T. Fadaly et al., Nature, vol. 580, p. 205, 2020.
[4] A. Li et al., Nanotechnology, vol. 34, p. 015601, 2022.
[5] S. Conesa-Boj et al., Nano Letters, vol. 17, p. 2259, 2017.
[6] M. Brauns et al., App. Phys. Lett., vol. 109, p. 143113, 2016.
[7] M. Brauns et al., Phys. Rev. B, vol. 94, p. 041411(R), 2016.

Germanium/Silicon Core Shell Nanowires for Spin/Hole Qubits Fabricated by Chemical Vapour Deposition

Nicolas Forrer[1], Arianna Nigro[1], Alicia Ruiz-Caridad[1], Gerard Gadea[1,2] and Ilaria Zardo[1,2]

[1]*University of Basel, Physics Department, Klingelbergstrasse 82, CH-4056 Basel.*
[2] *Swiss Nanoscience Institute, Klingelbergstrasse 82, CH-4056 Basel, Switzerland*

Tel: +41 61 207 55 90, Email: nicolas.forrer@unibas.ch

Ultra-clean germanium/silicon (Ge/Si) core shell nanowires (NWs) have been predicted and proven to host highly stable hole spin qubits, controllable via Rashba spin orbit interaction [1] with a large scalability potential, making it possible to develop realistic and reliable quantum computers [1,2]. To maximise their performance, high quality crystalline NWs grown along ⟨110⟩ direction [3] with well-defined Ge/Si interfaces are needed.
We present a detailed study on the growth kinetics of silicon (length 0.1–1 µm, diameter 10–60 nm) and germanium (length 0.06–1 µm, diameter 10–500 nm) NWs grown by chemical vapor deposition (CVD) applying the vapour–liquid–solid growth method catalysed by gold.
From these optimized CVD parameters, a reliable protocol was established to grow crystalline Ge NWs with the introduction of a low temperature (< 300 ºC) plasma enhanced deposition step for the Si shell. Using this approach, we were able to obtain fully crystalline Ge/Si core shell NWs, while avoiding the gold diffusion characteristic of high temperatures and responsible for shell contamination and disordered growth. The produced NWs exhibit Ge cores with diameters ranging from 5 to 30 nm, Si shells with thicknesses of up to 10 nm, defect free <110> axial nanowire growth direction and clean Ge/Si interfaces, as confirmed by electron microscopy. Furthermore, a processing technique was established to grow thin curved quantum wells to host hole spin qubits, using low temperature plasma enhanced growth conditions. This system is predicted to suppress charge noise, while keeping high coherence [4].

[1] C. Kloeffel, M. Trif, and D. Loss, Physical Review B **84**, 195314 (2011).
[2] C. Kloeffel, M. J. Rančić, and D. Loss, Physical Review B **97**, 235422 (2018).
[3] S. Conesa-Boj, A. Li, S. Koelling, M. Brauns, J. Ridderbos, T. T. Nguyen, M. A. Verheijen, P. M. Koenraad, F. A. Zwanenburg, and E. P. Bakkers, Nano letters **17**, 2259 (2017).
[4] S. Bosco and D. Loss, Phys. Rev. Appl., **18**, 044038 (2022)

Planar germanium quantum wells for hybrid semiconducting-superconducting quantum circuits

Daniel Chrastina, Oliver Sagi, Marco Valentini, Levon Baghumyan, Stefano Calcaterra, Andrea Ballabio, Marian Janik, Giorgio Fabris, Juan Aguilera Servin, Georgios Katsaros, Giovanni Isella

daniel.chrastina@polimi.it

Qubits based on hole spin in p-type Ge quantum wells have gained interested over the past few years, demonstrating long coherence with respect to electrons in GaAs and ease of fabrication and manipulation compared to electrons in Si. However, a dominant quantum computing technology approach is based on the transmon qubit realized using Josephson junctions between superconducting resonators. We discuss how Ge QWs grown by low-energy plasma-enhanced chemical vapour deposition (LEPECVD) are advantageous from a structural point of view, and also consider the material quality aspect. Key features of the structural profile are the thick forward-graded strain-relief buffer which provides a virtual substrate for the strained Ge QW, without requiring a thick buried Ge layer, and the thickness of the spacer layer between the Ge QW and the surface of the semiconductor.

Electrical Characterization of Hexagonal Silicon Germanium Nanowire

I. Bollier[1*], M. Vettori[2], W.H.J. Peeters[2], E.P.A.M. Bakkers[2], H. Schmid[1]

[1] IBM Research - Europe, [2] Eindhoven University of Technology
*isa@zurich.ibm.com

Silicon is the most important material for microelectronics, but its usefulness is limited in photonic or optoelectronic applications. In nature, silicon as well as germanium and its alloys crystalize in a cubic crystal structure and possess an indirect bandgap which suppresses the efficient emission of photons. Interestingly, $Si_{1-x}Ge_x$ alloys with x > 0.6 which crystalize in the metastable hexagonal crystal structure have a direct bandgap. TU Eindhoven (Tu/e) succeeded in growing wurtzite GaAs core nanowires (NWs) with hexagonal $Si_{1-x}Ge_x$ shells, and they subsequently measured their optical properties, showing excellent light emission capability.[1]
Ohmic contacts, especially low resistance ohmic contacts, are important for further device fabrication. In this work, we investigate the electronic contact formation and electrical characterization of two different hexagonal $Si_{0.2}Ge_{0.8}$ NWs growth runs. Metals with different work functions are used to contact the NWs (Figure 1a), and the influence of growth quality, doping, and post-annealing are investigated.

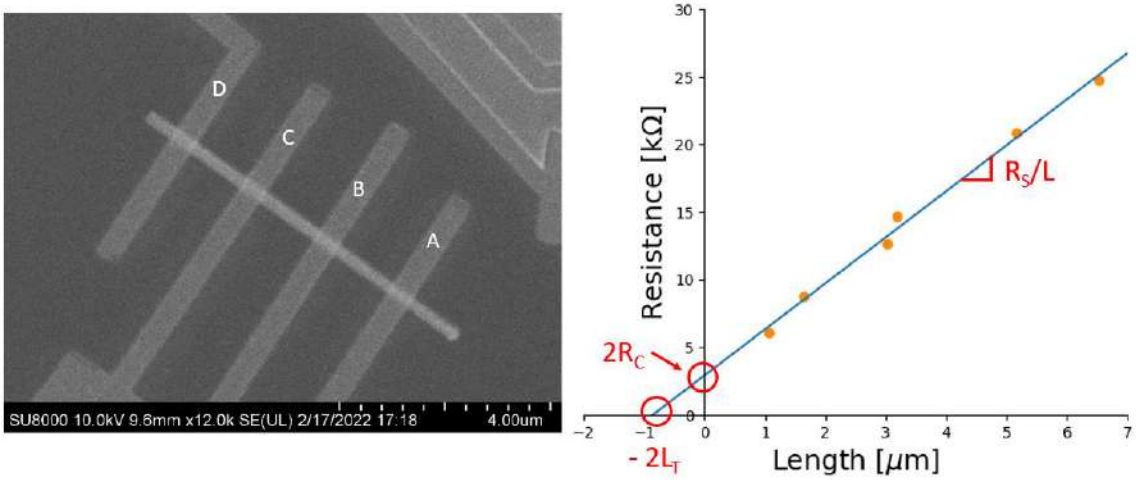


Figure 1. *a) SEM image of a contacted nanowire. b) TLM analysis to determine the contact and semiconductor resistivity.*

For the first batch of $Si_{0.2}Ge_{0.8}$ nanowires, two-point probe measurements persistently showed Schottky barriers. The barrier height does not change significantly using different metals (Ti, Ni, Pt and Al) for the contacts. Therefore, it is very likely that Fermi level pinning occurs at the metal/NW interface, as expected for n-doped cubic germanium.[2] However, after contact annealing, a linear I-V response is obtained indicating the formation of ohmic contacts.
For the second batch of $Si_{0.2}Ge_{0.8}$ nanowires, Tu/e managed to improve the crystal quality as well as to decrease the unintentional As (n-) doping during the growth. For the improved NWs, we obtained ohmic contacts independent of the used metal. By using the transfer line method (TLM) (Figure 1b), we could determine the semiconductor resistivity as well as the contact resistivity. Four-point probe measurements confirmed a resistivity of $3.7 \pm 0.2 \cdot 10^{-2}$ Ωcm for the hexagonal $Si_{0.2}Ge_{0.8}$ NWs.
We gratefully acknowledge technical support from the Binning & Rohrer Nanotechnology Center (BRNC) and funding from the European Union's Horizon 2020 research under the grant agreement No. 964191

References

[1] E.M.T. Fadaly; *Nature*, 2020, *580 (7802)*, 205-209.
[2] T. Nishimura; *Appl. Phys. Lett.*, 2007, *91 (12)*, 123123.

Growth of planar wurzite ZnS as a template for Hex-SiGe

Hassan MELHEM*[a], Vincent SALLET [b], Gaelle AMIRI [b], Géraldine HALLAIS [a], Charles PATRIARCHE[a], Nathaniel FINDLING[a], Charles RENARD[a], Laetitia VINCENT[a]

[a] University Paris-Saclay, CNRS, Center for Nanoscience and Nanotechnology, 91120 Palaiseau, France.

[b] University of Versailles Saint-Quentin-en-Yvelines, 78035 Versailles

* Hassan.melhem@c2n.upsaclay.fr

Historically, the formation of Ge-2H has been constrained to nanodomains via shear-induced phase transformation [1,2], core/shell nanowires [3,5,6], or more recently, nanobranches [7]. These methods inherently limit the active volume, impeding fundamental property investigations and device manufacturing. To address this limitation, there is a critical need to synthesize high-quality planar $Si_xGe_{(1-x)}$-2H crystals for scalable integration.

Wurtzite GaAs (GaAs-w) emerges as an ideal template for Ge-2H due to closely matched lattice parameters and thermal expansion coefficients. Demonstrating the feasibility of epitaxial growth, we utilized GaAs/Ge core/shell nanowires. Employing in situ transmission electron microscopy at the NANOMAX facility (Equipex TEMPOS), we established that, under specific growth conditions, a step-flow mode facilitates the perfect replication of the hexagonal structure of Ge-2H. These findings open up new possibilities for the epitaxial growth of $Si_xGe_{(1-x)}$-2H layers. Our objective is to employ wurtzite-type substrates with specific orientation and appropriate lattice parameters to pioneer the epitaxial growth of planar $Si_xGe_{(1-x)}$-2H layers.

In this study, we will present an investigation of ZnS wurzite epitaxy by MOCVD as a template for the synthesis of Ge wurzite by UHV-CVD. We will discuss the challenges encountered with other II-VI compounds such as CdS and introduce alternative approaches for forming $Cd_xZn_{(1-x)}S$ templates that would enable accommodation of the lattice parameters with Ge-2H.

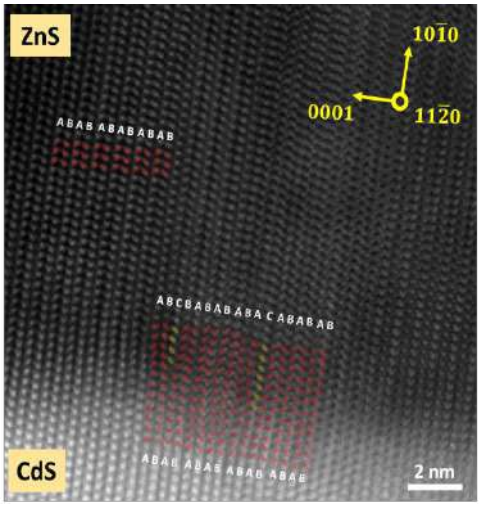


Figure 1: TEM image illustrating the ZnS template layer grown on a CdS-2H substrate by MOCVD, exhibiting a high-quality hexagonal layer with misfit dislocations.

[1]* Novel Heterostructured Ge Nanowires Based on Polytype Transformation
L. Vincent et al. Nano Letters 14 (2014) 4828 ;
[2]* Shear-driven phase transformation in silicon nanowires
L. Vincent et al. Nanotechnology 29 (2018) 125601 ;
[3] Direct-bandgap emission from hexagonal Ge and SiGe alloys
E. Fadaly et al. Nature 580 (2020) 205.
[4] Hexagonal Silicon Realized
***H.I.T.** Hauge et al.. Nano Lett. 15-9 (2015) 5855 ;*
[5] Growth-Related Formation Mechanism of I3-Type Basal Stacking Fault in Epitaxially Grown Hexagonal Ge-2H
L. Vincent et al. Adv. Mat. Inter. 9-16 (2022) 2102340
[6] Hexagonal Silicon-Germanium Nanowire Branches with Tunable Composition
A. Li et al. Nanotechnology 34-1 (2022) 015601 ;

INVITED

Opportunities and challenges in Group IV

Dan Mihai Buca
Forschungszentrum Jülich

The developing of new epitaxial group IV alloy has opened new opportunities for monolithical integration of functionalities, typically attributed to other material systems. One of them is efficient light emitters. Using GeSn alloys as gain medium optically and electrically pumped lasers have been developed lately. The latest developments and the prospect of the realization of electrically pimped Si-based lasers will be discussed. An important aspect is the power of epitaxy in realizing quantum heterostructure but also the creation of the ultimate group IV alloy the CSiGeSn. Using the large spectrum of Sn-based alloys, complicated heterostructures can be realize enabling large band-structure manipulation. Another field of application is the energy recovery. The epitaxial Sn-based alloys possess a low thermal lattice conductivity that may finally enable low heat recovery on chip.

University of Milano-Bicocca
Dept. of Materials Science

Development of data-driven machine learning interatomic potential for exploring pressure-dependent kinetics of phase transitions in Germanium

Andrea Fantasia, Emilio Scalise and Francesco Montalenti

Abstract

Understanding the pressure-dependent kinetics of phase transitions in materials is crucial for advancing various technological applications. In our recent research, we present the development of a data-driven machine learning interatomic potential (MLIP) tailored specifically for exploring the pressure-dependent kinetics of phase transitions in Germanium (Ge). Ge, with its allotropes, is of great technological interest. HD-Ge's predicted narrow direct band gap, for instance, renders it well-suited for optoelectronic applications compatible with silicon [1].

Germanium, with its allotropes, holds significant promise in various fields, making it an ideal system for such investigations.

To accurately reproduce such kinetic barriers, we incorporated configurations along minimum energy paths obtained through solid-state nudged elastic band (ssNEB) calculations under varying stress conditions into our training dataset. This approach ensures a comprehensive representation of transition mechanisms, including crucial saddle points defining kinetic barriers.

Our procedure is based on an active learning approach, involving multiple training of models on an iteratively refined training set, encompassing configurations sampled via NPT molecular dynamics and ssNEB calculations. The neural network potential was trained using the Deep Potential Molecular Dynamic package (DeePMD-kit) [2]. After training the model based on DFT-computed energies, forces, and stresses, we provide validation and we severely test the potential on unexplored paths. The resulting agreement with DFT calculations is remarkable in a wide range of pressures. The potential is exploited in large-scale NPT simulations, displaying local nucleation in the R8-Ge to β-Sn-Ge phase transformation, here taken as an illustrative example.
The resulting MLIP, demonstrates remarkable accuracy and efficiency, being several orders of magnitude faster than DFT calculations while scaling linearly with the number of atoms. Regression plots comparing MLIP-predicted properties with DFT calculations on a suitable test set showcase the robustness of our model in describing metastable allotropes of Ge and accurately predicting activation barriers.

Our work [3] not only presents a reliable MLIP for investigating pressure-dependent crystal phase transitions in Ge but also establishes a simple yet effective methodology for the iterative refinement of such models.

[1] E. M. T. Fadaly et al., "Direct-bandgap emission from hexagonal Ge and SiGe alloys," Nature, vol. 580, pp. 205–209, Apr. 2020.
[2] L. Zhang et al., "Deep Potential Molecular Dynamics: A Scalable Model with the Accuracy of Quantum Mechanics," Physical Review Letters, vol. 120, p. 143001, Apr. 2018.
[3] A. Fantasia et al., "Development of data-driven machine learning interatomic potential for exploring pressure-dependent kinetics of phase transitions in Germanium", (in preparation)

Growth and characterization of Ge/SiGe planar heterostructures for spin qubit applications

Arianna Nigro, Enrico Della Valle, Eric Jutzi, Alicia Ruiz-Caridad, Nicolas Forrer, Gerard Gadea, Vladimir Strokov, Andrea Hofmann, Ilaria Zardo

A great deal of interest is directed nowadays towards the development of innovative technologies in the field of quantum information and quantum computing, with emphasis in obtaining reliable qubits as building blocks. The realization of highly stable, controllable and accessible hole spin qubits is strongly dependent on the quality of the materials hosting them. Quantum wells (QWs) in ultra-clean germanium/silicon-germanium (Ge/SiGe) heterostructures have been predicted and proven to be the perfect candidates, and are opening the door towards the development of realistic and reliable solid state, all-electric quantum computers due to their large scalability potential.

The heteroepitaxial growth of SiGe layers with a high Ge content over Si wafers is challenging because of the large lattice mismatch between Si and Ge (~ 4.2%), which leads to the formation of misfit and threading dislocations. Therefore, the heterostructure has to be engineered and optimized to reduce the defect density.

The use of chemical vapor deposition (CVD) allows the epitaxial growth of thin films with high structural quality at elevated growth rates, compared to other techniques (e.g. molecular beam epitaxy, sputtering). The CVD growth conditions (temperature, pressure, flow rates of the gases, and growth time) influence dramatically the deposition rate and properties (crystallinity, interfaces quality, mobility) of the deposited layers. While this allows for a highly controllable process, the wide range of degrees of freedom makes it challenging and calls for a thoroughly optimization study.

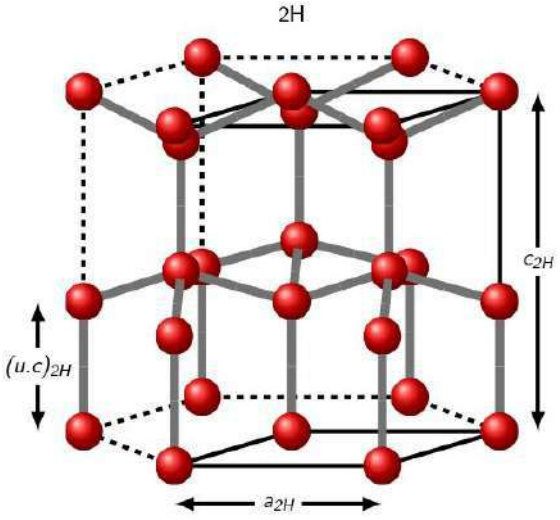
Engineering the design of Ge/SiGe heterostructures allows to control specific intrinsic physical properties of the materials involved. Optimization of the strain levels in the Ge QW allows to lift the degeneracy between the heavy holes and light holes states in the valence band, beneficial for spin qubits applications.

This work shows the results relative to the growth of epitaxial Ge/Si_{1-x} Ge_x heterostructures, using a reverse grading approach. In a first step, the CVD deposition kinetics and crystalline quality of the materials were investigated. In a second step, Raman spectroscopy and Soft X-ray ARPES were employed to quantitively measure the strain level and the HH-LH splitting in the QW.

Multiband $k \cdot p$ theory for hexagonal germanium — •Yetkin Pulcu[1], Janos Koltai[2], Andor Kormanyos[3], and Guido Burkard[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Department of Biological Physics, Eötvös Loránd University, Budapest, Hungary — [3]Department of Physics of Complex Systems, Eötvös Loránd University, Budapest, Hungary

The direct bandgap found in hexagonal germanium and some of its alloys with silicon allows for an optically active material within the group-IV semiconductor family with various potential technological applications. However, there remain some unanswered questions regarding several aspects of the band structure, including the strength of the electric dipole transitions at the center of the BZ. In this work [2], using 10 band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian with SOC near the Γ point, we obtain a self-consistent model that describes 2H-Ge via fitting to *ab initio* data. To understand the weak dipole coupling between the lowest conduction band and the top valance band, we start from a spinless 12-band model and show that when adding spin-orbit coupling, the lowest conduction band hybridizes with a higher-lying conduction band. Additionally, we derive the effective low-energy Hamiltonian for the conduction bands for the possible spin dynamics and nanostructure studies. Finally, we include the effects of a magnetic field and predict the electron and hole g-factor of the conduction and valence bands.

[1] Pulcu, Yetkin, et al. "Multiband $k \cdot p$ theory for hexagonal germanium." arXiv preprint arXiv:2310.17366 (2023).



INVITED

Tuning Electronic Properties of Hexagonal SiGe Quantum Wells

Silvana Botti
Ruhr Universität Bochum

We present accurate ab initio calculations of heterostructures comprising hexagonal Ge quantum wells embedded within direct-bandgap hexagonal SiGe layers. Our findings reveal a type-I band alignment in the heterostructures, with electron and hole wave functions localized in the Ge-richer regions. We observe that the quantum confinement of both charge carriers is notably influenced by interface orientation, well thickness, and internal and external strain. These results can be effectively interpreted using a rectangular potential-well model, with characteristic parameters derived from ab-initio band structures. Additionally, we discuss optical transition strengths alongside confinement energies and subbands.

[1] C. Roedl et al., Phys. Rev. Materials 3, 034602 (2019).
[2] E.M.T. Fadaly et al., Nature 580, 205 (2020).
[3] P. Borlido et al., Phys. Rev. Materials 5, 114604 (2021).
[4] A. Belabbes et al., Phys. Stat. Sol. RRL 16, 2100555 (2022).
[5] A. Belabbes et al. Phys. Rev. B 106, 085303 (2022).
[6] W.H.J. Wouters et al., submitted (2024).
[7] A. Belabbes et al., submitted (2024).

Ab initio modeling of n-type and p-type doping in hexagonal-diamond silicon

M. Túnica[1], A. Zobelli[1], M. Amato[1]

[1]Laboratoire de Physique des Solides, Université Paris-Saclay, CNRS, Orsay 91405, France, marc.tunica-i-rosich@universite-paris-saclay.fr.

Recent experiments showed that Si, whose bulk form presents a cubic-diamond structure (3C in the Ramsdell notation) at room temperature and atmospheric pressure, can show the diamond-hexagonal polytype (2H) (also know as lonsdaleite), if fabricated as nanowires [1,2]. These two polytypes present remarkably different structural and electronic properties. Indeed, while 3C-Si presents an indirect band gap of 1.12 eV with a minimum of the conduction band close to the X point, the 2H-Si polytype has a band gap of 0.95 eV with conduction band minimum in the M point.

Most of the fabricated 2H-Si samples present a high concentration of dopants whose effect on the electronic and optical properties has not been investigated yet. As a matter of fact, while defects in 3C-Si have been intensively studied in the past [3-6], only a few works in the literature have examined their role in 2H-Si [7,8].

Here we present results of ab initio DFT simulations in order to understand and describe the effect on the structural stability and on the electronic structure of p and n-type substitutional defects in 2H-Si. In particular, by studying ground state as well as charged systems using different DFT codes and approaches, we provide an accurate estimation of donor and acceptors transition energy levels in 2H-Si [9].

[1] E.M.T. Fadaly, A. Dijkstra, J.R. Suckert, et al. Nature, **2020,** 580, 205–209.
[2] S. Barth, M. S. Seifner, and S. Maldonado. Chemistry of Materials, **2020,** 32 (7), 2703-2741.
[3] M. Hakala, M. Puska and R. Nieminen, Phys. Rev. B, **2000**, 61, 8155–8161.
[4] M. Diarra, Y.-M. Niquet, C. Delerue and G. Allan, Phys. Rev. B: Condens. MatterMater. Phys. **2007**,75, 045301.
[5] I. Marri, E. Degoli and S. Ossicini. Phys. Status Solidi A. **2018**, 215, 1700414.
[6] L. E. Ramos, E. Degoli, G. Cantele, S. Ossicini, et al. J. Phys.: Condens. Matter **2007**,19, 466211.
[7] F. Fabbri, E. Rotunno, L. Lazzarini, D. Cavalcoli, et al. Nano Lett. **2013**, 13, 5900−5906.
[8] M. Amato, T. Kaewmaraya and A. Zobelli. The Journal of Physical Chemistry C **2020,** 124 (31), 17290-17298.
[9] M. Tunica, A. Zobelli and M. Amato (in preparation, 2024)

POSTER

Growth of hexagonal SiGe nano-branches

Denny Lamon[1], M. M. Jansen[1], M. A. Verheijen[1,2], E.P.A.M. Bakkers[1]

[1]Department of Applied Physics, Eindhoven University of Technology
[2]Eurofins Materials Science, High Tech Campus Eindhoven

Branched nanowires (Figure 1) offer a promising method for the controlled synthesis of hexagonal SiGe alloys with a high surface-to-volume ratio[1], holding potential for diverse applications. Axial heterostructures can be grown, leading to the possibility of fabricating electrically and optically addressable direct band gap *SiGe* quantum dots. Using the Metalorganic Vapor Phase Epitaxy technique, precise control over the growth of these branched nanowires is achievable by modulating the Si/Ge composition via the manipulation of precursors ratio and growth temperature. This approach enables the growth of more complex heterostructures including quantum wells and quantum dots, building blocks in the development of light-interacting quantum devices. But to do so, precise control over Si and Ge content is needed, as it directly influences the energy band gap of the material and consequently regulates the emitted light's wavelength[2]. However, achieving the desired Ge content necessitates meticulous tuning of the growth parameters, notably temperature and precursor ratio. Here we present an initial study on the influence of the temperature on the growth of *SiGe* branches. We observe that variations in temperature affect the morphology of the branches, altering their geometry, length, and tapering, as well as the Ge content in the material. Higher temperatures promote the incorporation of Si relative to Ge, resulting in a lower Ge content compared to the input provided during growth via the Si/Ge precursor ratio. A comprehensive investigation into growth parameters will enhance the control over the *SiGe* composition, opening the way for the fabrication of more complex heterostructures, such as Ge-rich quantum dots.

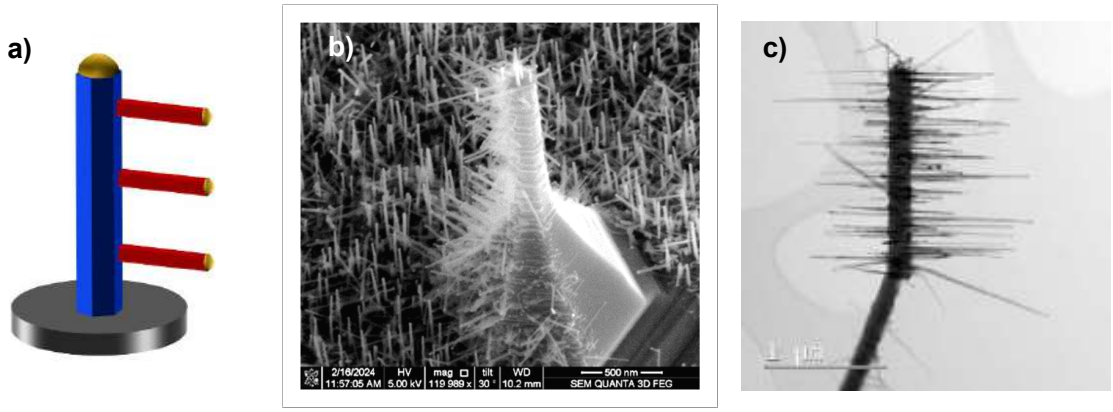


Figure 1: GaAs nanowire with SiGe branches: (a) Schematic illustration of the GaAs trunk (in blue) with the SiGe branches (in red). The Au catalyzing particles are visible at the end of the branches and at the top of the trunk. (b) SEM image of a SiGe branched GaAs nanowire with an input composition of 80%Ge. (c) TEM Image of branches and trunk along the [1-100] direction.

---

[1] Li A, Hauge HIT, Verheijen MA, Bakkers EPAM, Tucker RT, Vincent L, Renard C. Hexagonal silicon-germanium nanowire branches with tunable composition. Nanotechnology. 2022 Oct 12;34(1). doi: 10.1088/1361-6528/ac9317. PMID: 36126589.

[2] Fadaly, E.M.T., Dijkstra, A., Suckert, J.R. *et al.* Direct-bandgap emission from hexagonal Ge and SiGe alloys. *Nature* **580**, 205–209 (2020). https://doi.org/10.1038/s41586-020-2150-y

POSTER

High aspect ratio wurtzite GaAs nanowires as a platform for hexagonal SiGe

M.M. Jansen,[a] W.H.J. Peeters,[a] M.A. Verheijen,[a,b] and E.P.A.M. Bakkers[a]

[a] *Department of Applied Physics, Eindhoven University of Technology, Groene Loper 19, 5612AP Eindhoven, The Netherland*
[b] *Eurofins Materials Science BV, High Tech Campus 11, 5656 AE Eindhoven, The Netherlands*

The pursuit of constructing a silicon (Si) based laser has been akin to chasing the holy grail for numerous decades, as it signifies a crucial advancement in the journey towards making photonic circuits widely accessible for commercial use. One of the most promising pathways are the recently developed hexagonal silicon germanium (hex-SiGe) shells around wurtzite (WZ) gallium arsenide (GaAs) nanowires (NWs) for which efficient direct band gap emission was shown.[1] However, new studies have highlighted the limitations of the GaAs/SiGe core/shell NW system that notably restricts its lasing capabilities. These challenges include: the limitation of hexagonality induced by the formation of I3 defects,[2,3] the presence of Si concentration gradients in high-Si shells attributed to strain between the GaAs core and SiGe shell, as well as a recently discovered aspect ratio limitation in WZ GaAs NWs ascribed to a dynamic variation of the growth conditions.[4]
Here, we report on the crystal phase control of GaAs NWs down to the monolayer regime and towards high aspect ratios to improve the capabilities of GaAs/SiGe NWs. Therefore, Ga pulses are executed by momentarily halting the As supply, leading to an accumulation of Ga atoms within the catalyst particle. This process leads to the increase of the contact angle of the catalyst particle enabling a controlled transition from the WZ phase to the zinc blende (ZB), and then back to the WZ phase. This transition is analyzed in relation to the pulse duration and the diameter of the NW. By using the ZB inclusion as a marker during the growth process, we successfully carried out a detailed investigation into the evolution of the NW growth considering its diameter, length, and the pulse frequency. With this study, we pave the way for crystal phase control in high aspect ratio NWs with high crystal phase purity building an ideal platform for next generation hex-SiGe.

*presenting & corresponding author: Marvin Marco Jansen *e-mail: m.m.jansen@tue.nl

References:

1. Fadaly, E. M. T. *et al.* Direct-bandgap emission from hexagonal Ge and SiGe alloys. *Nature* **580**, 205–209 (2020).
2. Fadaly, E. M. T. *et al.* Unveiling Planar Defects in Hexagonal Group IV Materials. *Nano Lett* **21**, 3619–3625 (2021).
3. Vincent, L. *et al.* Growth-Related Formation Mechanism of I3-Type Basal Stacking Fault in Epitaxially Grown Hexagonal Ge-2H. *Adv Mater Interfaces* **9**, (2022).
4. Peeters, W. H. J. *et al.* Onset of uncontrolled polytypism during the Au-catalyzed growth of wurtzite GaAs nanowires. **020401**, 1–6 (2024).

POSTER

Infrared InAs nanowire lasers as a model system to compare with hexagonal-SiGe gain media.

S. Meder, B. Haubmann, F. del Giudice, P. Schmiedeke, J. Zöllner, G. Koblmüller, J. J. Finley.
Walter Schottky Institute and School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Extending the emission wavelengths of monolithically integrated nanowire (NW) lasers to longer wavelengths and even the mid-infrared (MIR) spectral range, 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 with wavelengths in the near- or mid-IR for low-loss optical transmission. While examples of NW lasers have been shown with emission in the near [1] to mid-infrared [2], few operate under continuous wave operation necessary for on-chip processors.

Here, we explore mid-infrared continuous wave lasing of individual InAs nanowires at cryogenic temperatures as a model system to compare with hexagonal-SiGe nanowires. Figure 1a shows finite difference time domain simulations of the diameter dependent threshold gain, that allow us to determine the optimal nanowire geometry (Fig. 1a). Catalyst-free InAs NWs are grown site-selectively and with high homogeneity on SiO_2-templated Si(111) substrates via molecular beam epitaxy, whereby the diameter and length is tuned from 160-745nm and 6-28µm by varying the pitch and growth durations (Fig 1c). Under optical pumping with a 976nm continuous wave laser, stimulated emission is demonstrated for individual NWs transferred on a sapphire substrate with diameters of 745±55 nm and nanowire resonator lengths between 10-30 µm (Fig 1b). Typical lasing thresholds are found to range from 2-30 kW/cm^2 with emission wavelengths of 2.4-2.7µm (0.455-0.515eV).

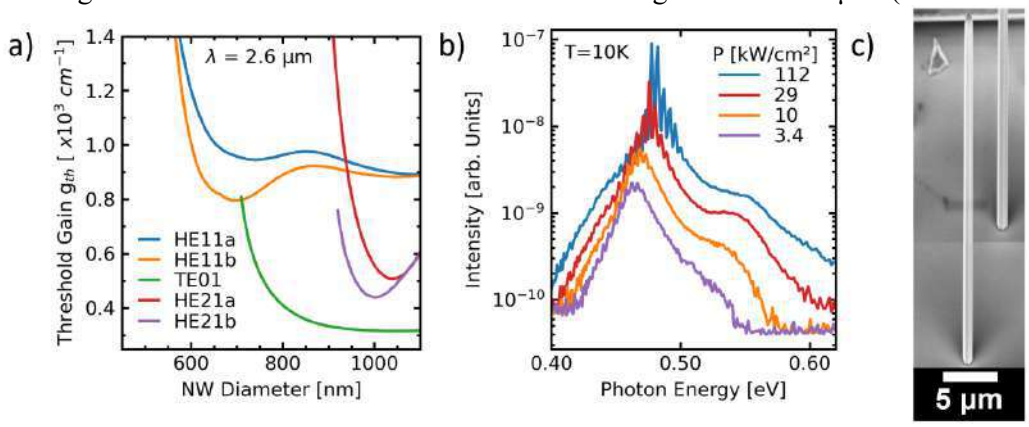


Figure 1 (a) FDTD simulations of the threshold gain for different guided modes, (b) Power dependent micro-PL spectra recorded from an individual InAs nanowire laser (c) SEM image of as grown InAs nanowires on silicon

+Corresponding Author Email: steffen.meder@wsi.tum.de

[1] P. Schmiedeke, et al., Appl. Phys. Lett. 118, 221103 (2021)
[2] H. Sumikura, et al., Nano Lett. 19, 8059 (2019)
[3] S. Meder, et al., in preparation (2024)

POSTER

Purcell-enhanced Quantum Emission using Hex-SiGe NW-induced Photonic Crystal Cavity

X. Wang,[a] J. Zöllner,[a] D. Liu,[a] S. Meder,[a] W. Peeters,[b] E. P. A. M. Bakkers,[b] J. Haverkort, [b] and J. J. Finley [a]

[a] *Walter Schottky Institute, School of Natural Science and Walter Schottky Institute, Technical University of Munich, Am Coulombwall 4, 85748 Garching, DE*

[b] *Department of Applied Physics, TU/e, Groene Loper 19, 5612AP Eindhoven, NL*

Semiconductor quantum dot (QD) is a promising platform for single photon emission [1]. Compared to cubic Si with low emission efficiency, hexagonal SiGe (hex-SiGe) alloys represent a new direct gap semiconductor that can be tuned 0.3 – 0.7 eV by tuning Ge content [2, 3]. Hence, hex-SiGe NWs with embedded QDs can serve as quantum light sources operating in mid infrared (MIR). The emission from single QDs requires external nanophotonic structures [4] for which the Purcell effect can be induced to enhance spontaneous emission [5] to manipulate the emission directionality and hence improve the collection efficiency of photons.

In this contribution, we demonstrate 2D silicon photonic crystals with a trench-like line defect, in which a SiGe NW is placed so that when there is QD embedded it behaves as an in-plane dipole source, as depicted schematically in figure 1(a). Cavity modes are self-localized in the photonic band gap of cavities with high quality factors (Q) exceeding several thousand and low modal volume (V_m). The cavity loss is primarily along the vertical direction allowing for efficient light-matter coupling to the QD. We optimised the radiation pattern and cavity metrics using finite difference time domain (FDTD) simulations by tuning geometrical parameters of the cavity. By shifting NW-QD along the trench relative to the unit cell of the photonic crystal we explore the impact on the cavity modes, as depicted in figure 1(b) and (c). We suggest that the moiré effect can be used for NWs containing multiple QDs separated by a distance that is incommensurate with the lattice periodicity.

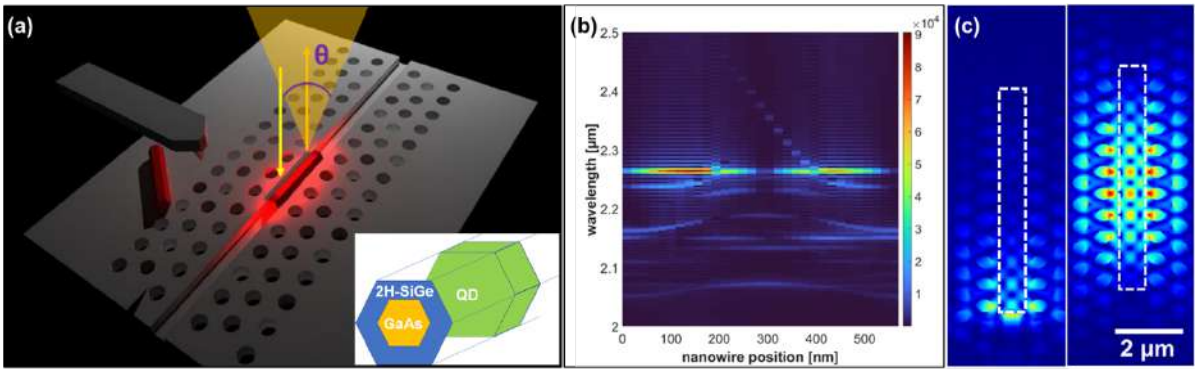


Figure 1: (a) Sketch of SiGe NW-induced PhC cavity. Image adapted from [6]. Inset: schematic of the GaAs-SiGe core-shell structure with a QD embedded. (b) Colourmap of cavity modes from FDTD simulation while shifting NW along the trench. (c) Electric field distribution from FDTD simulation revealing the NW shift effect.

[+]Corresponding Author Email: xuming.wang@wsi.tum.de

[1] C. L. Phillips et al. Sci. Rep. 14. 4450 (2024) [2] E. M. T. Fadaly et al. Nature 580.7802 (2020): 205-209 [3] X. Cartoixa et al. Nano Lett 17, 4753-4758 (2017) [4] I. Aharonovich et al. Nat. Phot. 10, 631-641 (2016) [5] O. Benson, Nature 480, 193-199 (2011) [6] M. Takiguchi et al. APL photonics 2.4 (2017)

POSTER

Towards Hanle effect measurements of electron and hole g-factors in hexagonal SiGe nanostructures

D.Liu,[a] X,Wang,[a] J. Zöllner,[a] S. Meder,[a] W. Peeters,[b] E. P. A. M. Bakkers,[b] Jos Haverkort[b] and J. J. Finley[a]

[a] *Walter Schottky Institute, School of Natural Science and Walter Schottky Institute, Technical University of Munich, Am Coulombwall 4, 85748 Garching, DE*

[b] *Department of Applied Physics, TU/e, Groene Loper 19, 5612AP Eindhoven, NL*

Silicon is highly attractive for semiconductor spin qubits due to its highly advanced nanofabrication technologies and the possibility to synthesize isotopically pure materials. On the other hand, photons are excellent carriers of quantum information since they propagate over very large distances and are only weakly perturbed by their environment. However, photons are difficult to store over long timescales and 2-qubit gates are difficult to achieve due to the weak optical non-linearities at the single photon level. It is, therefore, highly favorable to combine the advantages of scalability and stability of silicon technologies with the ability to light-matter coupling for control and for distributed quantum technologies. Cubic silicon has weak optical activity due to its indirect bandgap. However, direct bandgap hexagonal SiGe may offer a route to quantum photonic technologies on a silicon platform [1].

In this contribution we describe our efforts to measure g-tensors and understand the spin relaxation in hex-SiGe nanostructures using the Hanle effect [2]. Hereby, as shown by figure 1 a non-thermal spin population is induced by optical excitation using circularly polarized light. This leads to a degree of circular polarization of the emitted photoluminescence that reduces with applied magnetic field according to $\langle S_z(B)\rangle = \frac{\langle S_z(0)\rangle}{1+(\omega_L\tau^*)^2}$, where $\omega_L = g^*\mu_B B/\hbar$ is the Larmor frequency and τ^{*-1} is the generalized spin decay rate given by the sum of the radiative recombination and spin-relaxation rates ($\tau_*^{-1} = \tau_{rad}^{-1} + \tau_{spin}^{-1}$). Since τ_{rad}^{-1} has been recently shown to be $\sim 1\, ns^{-1}$ [1] and recent theory [3] has shown that $|g_h| = 17$ ($|g_e| = 1$) for hex-SiGe, we estimate that magnetic field strengths ~1-20mT will be required to depolarize the emission. We have constructed a MIR micro-PL setup allowing the measurement of Hanle curves for hex SiGe nanowires emitting close to 2.3µm. Hereby, a He-free cryostat-compatible magnetic coil system was designed using finite element simulations to produce B-fields of ~60mT, corresponding to Larmor frequency of 5 GHz for electrons and 95 GHz for holes.

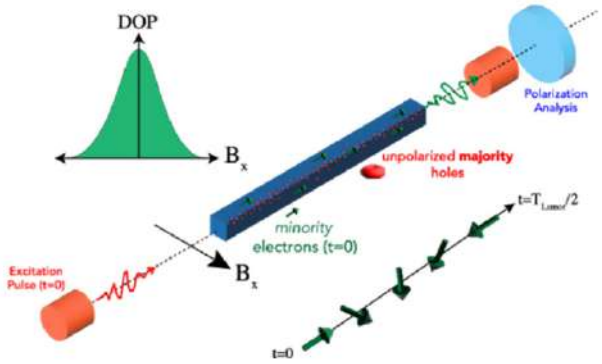


Fig 1 – Schematic representation of Hanle effect measurement. A magnetic field is applied perpendicular to the optical axis to depolarize the non-thermal spin population induced by optical pumping.

+Corresponding author: fingshan.liu@wsi.tum.de

[1] E. M. Fadaly et al, Nature580, 205–209 (2020), [2] H. Furthmeier et al. . Nature Comm. 7, 12413, (2016), [3] Y. Pulcu et al. arXiv:2310.17366

POSTER

Simulation and Fabrication of a Hex-SiGe NW-induced Photonic Crystal Cavity in Silicon

J. Zöllner,[a] S. Meder,[a] W. Peeters,[b] E. P. A. M. Bakkers,[b] G. Koblmüller,[a] J. J. Finley [a]

[a] *Walter Schottky Institute, School of Natural Science and Walter Schottky Institute, Technical University of Munich, Am Coulombwall 4, 85748 Garching, DE*

[b] *Department of Applied Physics, TU/e, Groene Loper 19, 5612AP Eindhoven, NL*

Semiconductor nanowires (NWs) represent a highly promising route to nanolasers for integrated silicon photonic circuits due to their potential for monolithic integration [1] as well as ultrafast modulation speeds arising from their sub-wavelength scale dimensions [2]. Naturally occurring cubic silicon has an indirect bandgap and is incapable of efficient light emission. In contrast, hexagonal silicon germanium (hex-SiGe) grown as a shell around a Wurtzite GaAs NW core has been recently shown to exhibit a direct bandgap for a Ge content higher than 67%. Variation of the Ge content allows tuning of the emission wavelength in a silicon transparent window between 1.8 and 3.4 µm [3]. On the road towards demonstrating an optically pumped hex-SiGe laser we demonstrate a NW self-induced photonic crystal cavity approach exploiting the formation of a localized mode confined in a NW, which is embedded in a trench between two hexagonal photonic crystals with air holes in silicon. The photonic crystal provides a high-Q cavity mode while simultaneously allowing the integration of the light source into the silicon photonics platform. The FDTD simulations presented in fig. 1 reveal that the cavity Q-factor exceeds 7200 at an emission wavelength of 2.2 µm for hex-$Si_{0.2}Ge_{0.8}$. Furthermore, as shown in figure 2 we established a fabrication process for the photonic crystal structure that facilitates precise control over the photonic crystal parameters as well as anisotropically etched sidewalls with low line edge roughness. The nanowires are inserted into the structure by a transfer printing method using polydimethylsiloxane (PDMS) polymer stamps with a sacrificial polycarbonate (PC) layer which allows precise positioning of single nanowires with sub-50 nm accuracy.

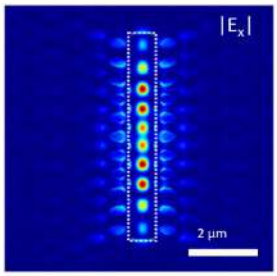


Figure 1 – FDTD simulation with high-Q localized mode

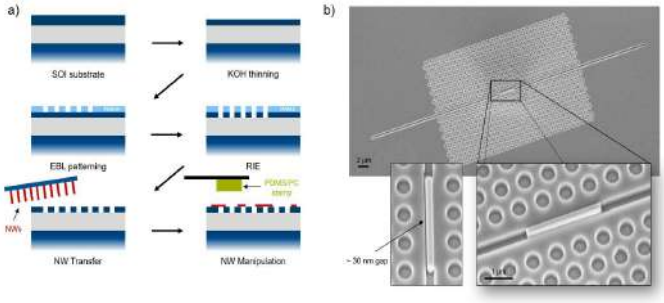


Figure 2 – a) Steps of the fabrication process b) SEM image of the NW-induced cavity

[+]Corresponding Author Email: jona.zoellner@wsi.tum.de

[1] Koblmüller et al, Semicond. Sci. Technol. 32 053001 (2017)
[2] Thurn et al, Phys. Rev. Applied 20, 034045 (2023)
[3] Fadaly et al, Nature580, 205–209 (2020)

POSTER

Growth of branched wurtzite GaAs nanowire for Hybrid III-V/IV heterostructures.

H.A.J. van der Donk,[a] D. Lamon,[a] M.M. Jansen,[a]
M.A. Verheijen,[a,b] J.E.M. Haverkort,[a] and E.P.A.M. Bakkers[a]

[a] *Department of Applied Physics, Eindhoven University of Technology, Groene Loper 19, 5612AP Eindhoven, The Netherland*

[b] *Eurofins Materials Science BV, High Tech Campus 11, 5656 AE Eindhoven, The Netherlands*

The widespread use of silicon in current semiconductor technologies favors silicon-based components for integration. Due to the direct bandgap nature of hexagonal Silicon-Germanium(hex-SiGe),[1] it poses a platform for integrated optoelectronics and quantum computing. Current approaches to fabricating hex-SiGe involve growing an hexagonal crystal structure material such as Gallium Arsenide (GaAs) nanowires (NWs), and growing SiGe on top, transferring its crystal structure. This is done either by vapor-solid core/shell growth,[1] or has also been done using a vapor-liquid-solid (VLS) branch growth approach.[2] The latter method uses a second deposition of Au after the wire is grown, forming catalyst particles after an annealing step. This stochastic process however gives limited control in the amount and size of catalyst particles and thus SiGe branches.

Here, we show a strategy for gaining control in branch growth by creating branched wurtzite (WZ) GaAs NWs by catalyst destabilization which is utilized as a template for single hex-SiGe branches. The process of destabilization, wherein the catalyst favors wetting a side facet instead of the top facet as seen in figure 1a), is explored and optimized to have both a high yield of NWs and destabilized catalysts. Next, a WZ GaAs branch is grown in the radial direction of the NW as seen in figure 1b). The quality of the hexagonal crystal structure is verified using transmission electron microscopy. The branched WZ GaAs NW, called 'starter' forms an hexagonal template from which a hex-SiGe heterostructure can be grown by VLS growth. The precise control of the starter forms a unique opportunity to adjust the subsequent growth of the SiGe branch morphology to enable complex heterostructures.

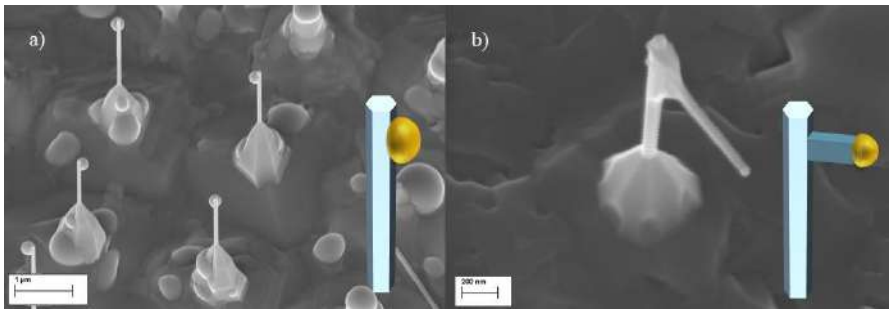


Figure 1: a) GaAs NW after destabilization of the Au catalyst. The droplet is wetting a side facet of the wire. b) GaAs branch growth from a destabilized particle. The Au catalyst is at the end of the branch.

[1] Fadaly, E. M., *et al.* (2020). Direct-bandgap emission from hexagonal Ge and SiGe alloys. *Nature*, *580*(7802), 205-209.

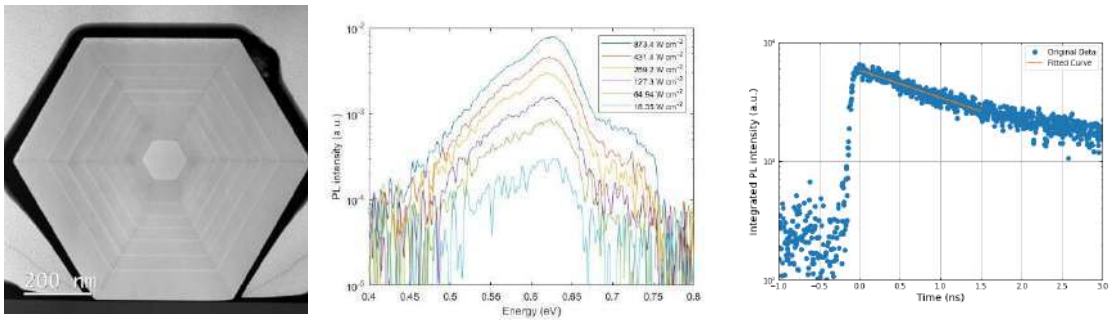
[2] Li, A., *et al* (2023). Hexagonal silicon−germanium nanowire branches with tunable composition. *Nanotechnology* 34 015601

POSTER

Carrier Dynamics in Hex-SiGe Quantum Wells (poster)

Cristian Wakelkamp, Riccardo Farina, Wouter H.J. Peeters, Erik P.A.M. Bakkers, Jos E.M. Haverkort

Silicon (Si) is dominant in semiconductor technology [1]. To further develop computing technologies it is essential to create a Si based laser [2]. However, cubic-Si and germanium (Ge) are indirect semiconductors implying that they cannot emit light efficiently and therefore a Si-based laser is still missing. In 2020, it was shown that a direct bandgap material can be created with hexagonal silicon germanium (hex-SiGe) resulting in efficient light emission [3]. The lasing threshold of hex-SiGe can be lowered by integrating quantum well (QW) structures in the material. Here, the emission characteristics of hex-SiGe multiple quantum wells (MQW) nanowires (NWs) are presented. A TEM cross-section of one of the NWs containing six QWs can be observed in Fig. 1a. As-grown hex-$Si_{0.1}Ge_{0.9}/Si_{0.3}Ge_{0.7}$ MQW NWs were investigated using Fourier transform Infrared (FTIR) based spectral photoluminescence (PL) measurements. The QWs consist of $Si_{0.1}Ge_{0.9}$ and the barrier of $Si_{0.3}Ge_{0.7}$. In Fig. 1b, the emission spectrum of the as grown hex-$Si_{0.1}Ge_{0.9}/Si_{0.3}Ge_{0.7}$ MQW NWs as a function of the excitation density is shown. Furthermore, time-resolved photoluminescence (TRPL) measurements were performed on single hex-$Si_{0.1}Ge_{0.9}/Si_{0.3}Ge_{0.7}$ MQW NWs to measure the spectral and temporal information. The integrated PL intensity over time is shown in Fig. 1c. Fitting the lifetime using a mono-exponential decay fit results in a lifetime of 1.89±0.04 ns. Thus, we prove that MQW are a promising solution to effectively lower the laser threshold and therefore achieving lasing.



a) b) c)

Figure 1 a) TEM cross-section of a hex-$Si_{0.1}Ge_{0.9}/Si_{0.3}Ge_{0.7}$ MQW NW containing six QWs. b) Emission spectrum from as-grown hex-$Si_{0.1}Ge_{0.9}/Si_{0.3}Ge_{0.7}$ MQW NWs at different excitation densities on a logarithmic scale. c) The integrated PL intensity of the QW emission on a logarithmic scale as a function of the time. The solid orange line is an exponential fit applied on the integrated PL intensity resulting in a lifetime of 1.89±0.04 ns.

[1] Kamal, K. Y. (2022). The Silicon Age: Trends in Semiconductor Devices Industry. *Journal of Engineering Science & Technology Review*, *15*(1).

[2] Miller, D. A. (2000). Optical interconnects to silicon. *IEEE Journal of Selected Topics in Quantum Electronics*, *6*(6), 1312-1317.

[3] Fadaly, E. M., *et al.* (2020). Direct-bandgap emission from hexagonal Ge and SiGe alloys. *Nature*, *580*(7802), 205-209.

POSTER

Toward the formation of 2H Germanium by HPHT conditions with in-situ FIR probe

Pierre Hemme, **Marine Verseils**, Jean-Blaise Brubach, Pascale Roy, Charles Renard, Laetitia Vincent

Germanium is a material of high interest in the field of semiconductors due to its electronic and optical properties. At ambient conditions of pressure and temperature the Ge is cubic, and its common use exploits its bandgap in the Near-IR (0.7 eV). Recently, the scientific community has intensified research efforts to obtain hexagonal 2H Ge, whose optical properties are predicted to be energetically favorable (optical direct bandgap of 0.3 eV compared to the 0.7 eV indirect bandgap of cubic germanium).

The work presented here, resulting from a collaboration between the SEEDS team at C2N and the AILES beamline at the SOLEIL Synchrotron, comes from the prediction of a theoretical article in which the transition from cubic to hexagonal germanium is calculated at pressures higher than 80 GPa **[1]**. Moreover, Pandolfi et al. show that cubic Si transits into a 4H structure using high-temperature and high-pressure multi-anvil synthesis **[2]**. We decided to combine high-pressure and high-temperature (HP-HT) with Far-Infrared Fourier transformed (FT-IR) spectroscopy to observe *in-situ* the transition from the cubic phase to the desired 2H phase of a massive germanium sample and obtain the phonon signature of each phase of the P-T phase diagram. This was possible thanks to the specific set-up available of the AILES beamline of synchrotron SOLEIL.

We measured a disc of cubic germanium with 250 microns of diameter and a thickness of 60 microns that we compressed in a diamond anvil cell (DAC) filled with argon. The cell was placed in a vacuum chamber and encapsulated in a heating ring. First, we obtained for the first time the Far-IR spectrum of the ST-12 tetragonal phase of Ge by performing a compression/ decompression cycle at room temperature (see Figure 1.a). Secondly, by combining high temperature and a compression-decompression cycle, we succeeded in obtaining a new transient phase different from the well-known ST-12 and metallic β-tin. This unknown phase is characterized by three peaks at 150 cm^{-1}, 285 cm^{-1}, and 425 cm^{-1} in the Far-IR spectrum (see Figure 1.b).

Further experiments are necessary to confirm the appearance of the new phase and try another pressure/temperature return path to stabilize it at ambient conditions. Additionally, to HP-HT FT-IR in DAC environment, we will try to synthesize this phase using a large multi-anvil press available at IMEM-CNR (Parma) combined with high temperature. This will permit to obtain bigger quantity of product to analyze the new phase with complementary techniques (DRX, …).

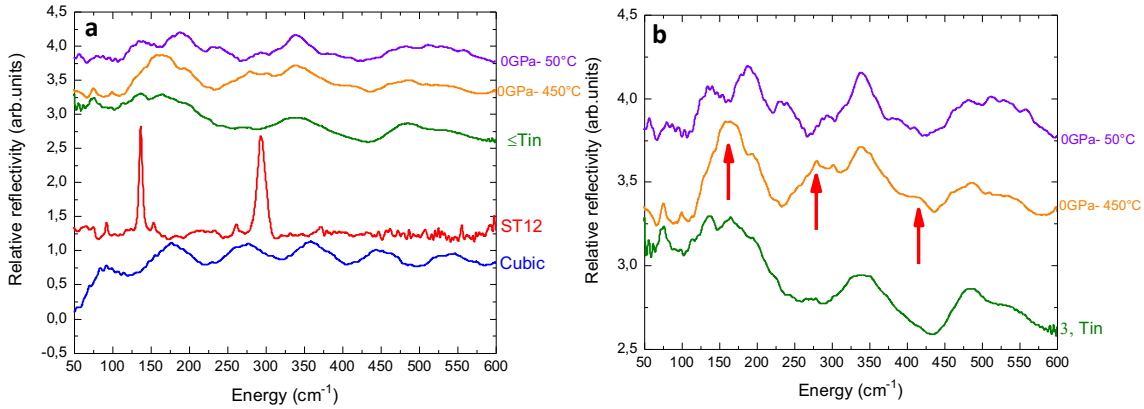


Figure 1 : Infrared spectra of Ge sample obtained during the P-T cycle performed on the AILES beamline

[1] : Katzke *et al.*, Phys. Rev. B 73, 134105

[2] : Pandolfi *et al.*, Nano Lett. 2018, 18, 9, 5989–5995

POSTER

Growing SiGe nanowires with the hexagonal phase

H. Ameziane, H. Melhem, G. Patriarche, T. Van den Berg, G. Hallais, C. Renard, L. Travers, L. Vincent

Université Paris-Saclay, CNRS, Centre de Nanosciences et de Nanotechnologies,91120 Palaiseau, France

We previously reported that Au catalyzed Ge-2H branches [1] can grow on the sidewalls of a GaAs wurtzite trunck nanowires with the particular direction <1-100> as shown in figure 1. The Ge nanobranches exhibit the crystal structure 2H under the Au catalyst (i.e. epitaxial relationship with the (1-100) sidewalls of the GaAs trunks). An additional lateral layer of cubic Ge (3C) may grow on the (0001) facets depending on growth conditions (Fig .1).

Based on these observations, our objective is to grow hexagonal GeSi nanowires by UHV-CVD on wurtzite bulk substrates with m-plane (1-100) surface. As GaAs with a bulk wurtzite phase does not exist, we have opted for alternative hexagonal substrates with m-plane surfaces and lattice parameters corresponding to those of Si and Ge such as CdS-2H and ZnS-4H. We have studied the dewetting of the Au catalyst on these substrates and determined the optimal parameters for the growth of hexagonal SiGe nanowires.

Figure 1: 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.

[1] A Li et al (2023). Hexagonal Silicon-Germanium nanowire branches with tunable composition. Nanotechnology, 34 015601

POSTER

Characterizing Optical Cavities in hex-SiGe Nanowires

Riccardo Farina[1], Marvin A.J. van Tilburg[1], Victor T. van Lange[1], Wouter H.J. Peeters[1], Steffen Meder[2], Marvin M. Jansen[1], Jos. E.M. Haverkort[1], Erik. P.A.M. Bakkers[1]

[1] *Eindhoven University of Technology, Eindhoven, Netherlands*
[2] *Technical University of Munich, Munich, Germany*
Presenting author: Riccardo Farina (r.farina@tue.nl)**.** Poster presentation is preferred.

The integration of hexagonal SiGe (hex-SiGe) into the semiconductor industry requires the development of miniaturized components capable of emitting laser light. To achieve lasing with hex-SiGe, nanowires (NWs) are a promising approach due to their natural behavior as Fabry-Perot resonator cavities. Although amplified spontaneous emission (ASE) has been recently observed in hex-SiGe nanowires, the demonstration of strong and stable lasing remains elusive.
In this study we make use of the procedure presented by Liu et al.[1] for assessing the quality of NWs as Fabry-Perot cavities by measuring the linewidth of the ASE spectrum.
Single NWs are placed on the edge of a substrate to increase the end-facet reflectivity (Fig. A, B) and they are measured in a Time-Resolved Fourier Transform Infrared Spectroscopy setup.
The resonance peaks are then isolated from the total spectrum and the interferogram is retrieved by performing an inverse Fourier transform (see Fig. C,D). The Full Width Half Maximum (FWHM) of the interferogram corresponds to the coherence length of the emission.
Our findings with 7 µm nanowires demonstrate a coherence length of 160 µm, indicative of a cavity lifetime of 0.08 ps, end facet reflectivity exceeding 41%, and absorption losses below 1370 cm^{-1}. These results confirm that the Fabry-Perot cavities in hex-SiGe nanowires exhibit high reflectivity and low intrinsic losses. Utilizing these findings, we estimate an optical modal gain of approximately -500 cm^{-1} for hex-SiGe using the Hakki-Paoli method.[2]
In conclusion, the optical cavity quality of hex-SiGe NWs is comparable to many III-V semiconductor NW lasers. However, lasing is not yet achieved due to insufficient round-trip gain. Our study, particularly the calculated optical modal gain, is crucial for overcoming these challenges and enabling stable lasing, which would be a significant advancement for hex-SiGe in integrated photonics.

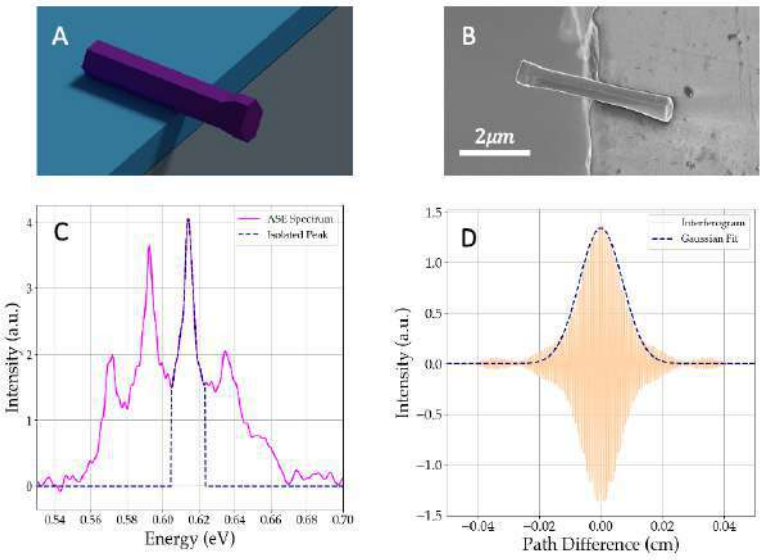


Figure: (A) schematic view of the nanowire on the substrate edge, (B) SEM picture of a measured NW, (C) ASE spectrum of a single NW. The blue dashed line represents the isolated resonance peak, (D) computed interferogram of the isolated resonance peak. The amplitude is fitted with a gaussian function (dashed line).

[1] Yuanda Liu et al., Room temperature nanocavity laser with interlayer excitons in 2D heterostructures. Sci. Adv.5,eaav4506(2019).DOI:10.1126/sciadv.aav4506
[2] M. Vanzi, G. Marcello, G. Mura, G. Le Galès, S. Joly, Y. Deshayes, L. Bechou, Practical optical gain by an extended Hakki-Paoli method, 2017, https://doi.org/10.1016/j.microrel.2017.07.060.

POSTER

Lifetime and Optical Matrix Element of Hexagonal Ge

V.T. v. Lange[1,*], A. Dijkstra[1,2], E.M.T. Fadaly[1], W.H.J. Peeters[1], M.A.J. v. Tilburg[1], E.P.A.M. Bakkers[1], J.E.M. Haverkort[1]

[1]Department of Applied Physics, Eindhoven University of Technology, Groene Loper 19, 5612AP Eindhoven, The Netherlands, [2]Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching, Munich, Germany.

** Presenting author, Email: v.t.v.lange@tue.nl*

The hex-$Si_{1-x}Ge_x$ nanowire material system provides a new direct bandgap semiconductor which is promising for Si-compatible lasers and optical amplifiers [1]. Due to the change in crystal structure from cubic to hexagonal, a direct bandgap emerges as the L-point is folded towards the Γ-point [2]. For hex-Ge however, theoretical calculations predict a very long 20µs radiative lifetime [1,2]. A short radiative lifetime is a requirement for efficient light emission, and while hex-$Si_{0.2}Ge_{0.8}$ has experimentally been shown to feature a subnanosecond radiative lifetime [1], measurements of the lifetime of hex-Ge remain challenging due to lack of available detectors and the blackbody radiation background.

We leverage an extended Lasher-Stern-Würfel (LSW) model[3,4] fitting it to low temperature (4K) photoluminescence spectra as a function of excitation density with great agreement as shown in Fig. 1. The model gives direct access to the steady-state carrier distributions which, when combined with the generation rate, can be used in a rate equation model to calculate the carrier lifetime. Given that hex-SiGe is shown to be in the radiative limit at 4K and hex-Ge is of similar optical quality [1], we find a radiative lifetime of τ=1.7ns which is in stark contrast to the predicted 20µs [2]. Moreover our model also provides an estimation for the optical transition strength derived from the absorption strength. Here we find a matrix element in the form of the transition's Kane energy $E_K \geq 3.06eV$ which greatly exceeds the $E_K \approx 0.002eV$ expected for a pseudo-direct bandgap by [2].

In conclusion we observe a (favorable) discrepancy between theory and experiment for hex-Ge, where theory predicts a slow lifetime of 20µs and a low Kane energy while the LSW fits to the experiment show both a high Kane energy and a nanosecond radiative lifetime. This implies that hex-Ge allows bright light emission and promises to be a suitable material for hex-Ge lasers as well as a building block for active optical components in silicon integrated opto-electronics.

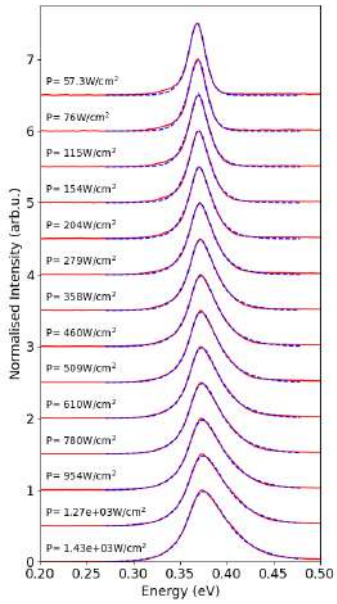


Figure 1: Measured photoluminescence (PL) spectrum of hex-Ge between 75.3 W/cm² and 1.43 kW/cm² fitted with the Lasher-Stern-Würfel (LSW) model

[1] E.M.T. Fadaly et al., "Direct-bandgap emission from hexagonal Ge and SiGe alloys," Nature, vol.580, no.7802, pp.205–209, Apr.2020.

[2] C. Rödl, et al, "Accurate electronic and optical properties of hexagonal germanium for optoelectronic applications," Phys. Rev. Mater., vol.3, no.3, 2019.

[3] G. Lasher and F. Stern, "Spontaneous and stimulated recombination radiation in semiconductors," Phys. Rev., vol.133, no.2A, p.A553, Jan.1964.

[4] P. Wurfel, "The chemical potential of radiation," J. Phys. C Solid State Phys., vol.15, no.18, pp.3967–3985, Jun.1982.

POSTER

Accelerating simulations of strained Ge surfaces evolution via Machine Learning

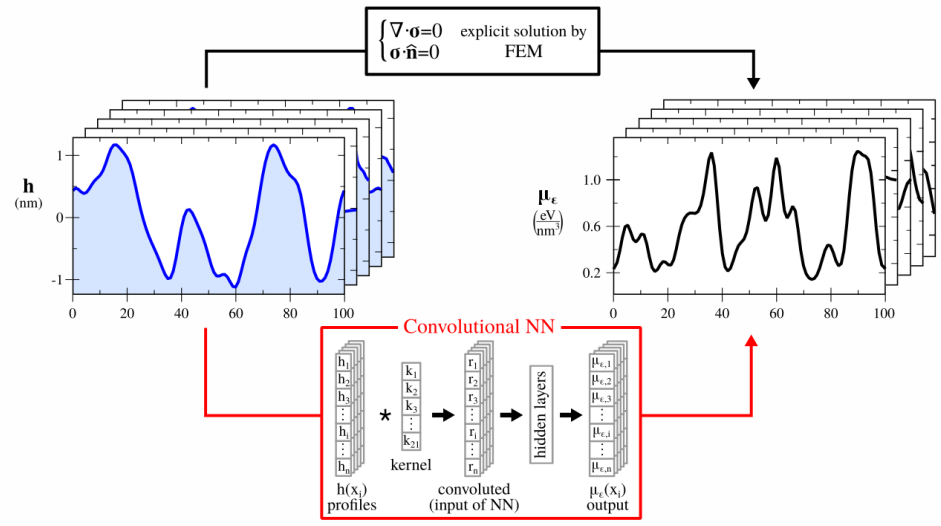
D. Lanzoni[a], F. Rovaris[a], L. Martìn Encinar[b], A.Fantasia[a], R. Bergamaschini[a], and F. Montalenti[a]

[a] L-NESS and Dept. of Materials Science, Università degli Studi di Milano – Bicocca, Milano, Italy
[b] Dpto. de Electricidad y Electrónica, E.T.S.I. de Telecomunicación, Universidad de Valladolid, 47011, Valladolid, Spain

In recent years Machine Learning has proven to be an attractive tool to accelerate materials simulations [1]. Methods such as Neural Networks allow for the automatic learning of fast approximations for the most computationally demanding steps while maintaining high accuracy. This family of schemes has proven to be particularly effective in atomistic simulations [2]. Applications to continuum models, however, are less common [3]. We here present a proof of concept in this direction, specializing this general framework to the simulations of the morphological evolution and growth of strained Ge films in a 2D, isotropic approximation on a continuum level.

In the context of continuum models for strained free–surfaces, one of the main driving forces is the elastic energy density. In traditional simulation workflows, tracking a full evolution could require several hundred thousand Finite Element Method (FEM) calls [4], which is currently one of the main bottlenecks for high throughput simulations of surface evolutions. We show that explicit FEM calculations can be substituted with a Convolutional Neural Network (CNN) predicting the elastic energy density for an arbitrary profile. Importantly, we discover that a dataset of only ~70’000 FEM calculations is sufficient to obtain substantial generalization capabilities. At the same time, computational costs are compressed by several orders of magnitudes, allowing extensive studies while retaining a high level of accuracy.

Future extensions integrating plastic relaxation mechanisms, anisotropy and a full 3D description of the free surface are envisioned.



[1] Zdeborová, Lenka. "New tool in the box." Nature Physics 13.5 (2017): 420-421.
[2] Hellström, Matti, and Jörg Behler. "Neural network potentials in materials modeling." Handbook of Materials Modeling: Methods: Theory and Modeling (2020): 661-680.
[3] Lanzoni, Daniele, et al. "Morphological evolution via surface diffusion learned by convolutional, recurrent neural networks: Extrapolation and prediction uncertainty." Physical Review Materials 6.10 (2022): 103801.

[4] Rovaris, Fabrizio, Roberto Bergamaschini, and Francesco Montalenti. "Modeling the competition between elastic and plastic relaxation in semiconductor heteroepitaxy: From cyclic growth to flat films." Physical Review B 94.20 (2016): 205304.